ANSWER 1 OF 40 CAPLUS COPYRIGHT 2000 ACS

1999:733038 CAPLUS ΑN

131:351343 DN

Preparation of heterocyclic compounds for the treatment of diabetes and ΤI related diseases

Lohray, Vidya Bhushan; Lohray, Braj Bhushan; Paraselli, Rao Bheema; ΙN Gurram, Ranga Madhavan; Ramanujam, Rajagopalan; Chakrabarti, Ranjan; Pakala, Sarma K. S.

Reddy's Research Foundation, India; Reddy-Cheminor Inc. PΑ

U.S., 35 pp., Cont.-in-part of U.S. 5,885,997. SO CODEN: USXXAM

Patent DT

English LA

FAN.	CNT 3 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI PRAI	US 5985884 US 5885997 IN 1996-DE1150 US 1996-777627	A A 19960 19961		US 1997-884816 US 1996-777627	19970630 19961231
OS GI	MARPAT 131:35134	3			

$$R^{1}$$
 X
 X
 Z
 $Y+N$
 $[CH_{2}]_{\overline{n}}O-Ar$
 A
 A
 B
 N
 H
 O
 I

The title compds. [I; one of X, Y, Z = C(O), C(S) and one of the remaining of X, Y, Z = C and the other C:C; R1-R3 = H, halo, OH, etc.; n = 1-4; Ar 703-308-4488 Searched by John Dantzma

QAZI

(un) substituted divalent aryl, heteroaryl; R4 = H, halo, alkyl or forms a bond together with the adjacent group A; A = N, CR5 (wherein R5 = H, halo,

alkyl or R5 forms a bond together with R4); B = O, S when A = CR5 and B =O when A = N], novel antidiabetic compds., were prepd. and formulated. Thus, reacting 4-[2-(2-ethyl-4-methyl-6-oxo-1,6-dihydro-1-

pyrimidinyl)ethoxy]benzaldehyde (prepn. given) with

thiazolidine-2,4-dione

afforded II which showed 67% max. redn. in blood glucose level at 100 mg/kg/day (6 days treatment) in mice.

199114-24-4P 199114-25-5P 199114-26-6P ΙT 199114-27-7P 199114-28-8P 199114-29-9P 199114-30-2P 199114-31-3P 199114-32-4P 199114-33-5P 199114-34-6P 199114-35-7P 199114-36-8P 199114-37-9P 199114-38-0P 199114-39-1P 199114-40-4P 199114-41-5P 199114-42-6P 199114-43-7P 199114-44-8P 199114-45-9P 199114-46-0P 199114-47-1P 199114-48-2P 199114-51-7P 199114-52-8P

199114-54-0P 199114-55-1P 199114-56-2P

199114-57-3P 199114-59-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of heterocyclic compds. for the treatment of diabetes and related diseases)

RN 199114-24-4 CAPLUS

Benzaldehyde, 4-[2-(4-methyl-6-oxo-2-propyl-1(6H)-pyrimidinyl)ethoxy]-CN (CA INDEX NAME)

199114-25-5 CAPLUS RN

Benzaldehyde, 4-[2-(2,4-dimethyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]- (9CI) CN (CA INDEX NAME)

199114-26-6 CAPLUS RN

Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{N---} \text{CH}_2\text{---} \text{CH}_2 \\ \text{O} \\ \end{array} \begin{array}{c} \text{CHO} \\ \end{array}$$

RN 199114-27-7 CAPLUS CN Benzaldehyde, 4-[2-(2-butyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-28-8 CAPLUS
CN Benzaldehyde, 4-[2-[4-methyl-6-oxo-2-(phenylmethyl)-1(6H)-pyrimidinyl]ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-29-9 CAPLUS
CN Benzaldehyde, 4-[2-(2,5-diethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy](9CI) (CA INDEX NAME).

Me
$$N$$
 N CH_2 CH_2 O CHO

RN 199114-30-2 CAPLUS CN Benzaldehyde, 4-[2-(2-ethyl-6-oxo-4-phenyl-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

199114-31-3 CAPLUS RN

Acetamide, N-[1-[2-(4-formylphenoxy)ethyl]-1,2-dihydro-2-oxo-4-CN pyrimidinyl] - (9CI) (CA INDEX NAME)

199114-32-4 CAPLUS RN

Benzaldehyde, 4-[2-(4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX CN NAME)

199114-33-5 CAPLUS RN

Benzaldehyde, 4-[2-(2-methyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA CN INDEX NAME)

199114-34-6 CAPLUS RN

Benzaldehyde, 4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA CN INDEX NAME)

RN 199114-35-7 CAPLUS

CN Benzaldehyde,

4-[2-(2-methyl-4-oxopyrido[2,3-d]pyrimidin-3(4H)-yl)ethoxy](9CI) (CA INDEX NAME)

RN 199114-36-8 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]- (9CI) (CA INDEX NAME)

RN 199114-37-9 CAPLUS

CN Benzaldehyde, 4-[(3-ethyl-3,4-dihydro-4-oxo-2-quinazolinyl)methoxy]-(9CI)

(CA INDEX NAME)

RN 199114-38-0 CAPLUS

CN Benzaldehyde, 4-[(1,4-dihydro-1-methyl-4-oxo-2-quinazolinyl)methoxy](9CI) (CA INDEX NAME)

Searched by John Dantzma 703-308-4488

RN 199114-39-1 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]-3-methoxy- (9CI) (CA INDEX NAME)

RN 199114-40-4 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, 1-oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{N} \\ \text{O} \end{array} \quad \begin{array}{c} \text{CH} \\ \text{CH} \\ \text{N} \\ \text{OH} \end{array}$$

RN 199114-41-5 CAPLUS CN 4(3H)-Pyrimidinone,

2-ethyl-3-[2-[4-[(hydroxyamino)methyl]phenoxy]ethyl]-6methyl- (9CI) (CA INDEX NAME)

RN 199114-42-6 CAPLUS

CN Urea,

N-[[4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]phenyl]met Searched by John Dantzma 703-308-4488 hyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 199114-43-7 CAPLUS CN 4(3H)-Pyrimidinone, 2-ethyl-6-methyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

RN 199114-44-8 CAPLUS CN 4(3H)-Quinazolinone, 2-ethyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

RN 199114-45-9 CAPLUS CN 4(3H)-Pyrimidinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl-6-methyl- (9CI) (CA INDEX NAME)

RN 199114-46-0 CAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl- (9CI) (CA
INDEX
NAME)

$$\begin{array}{c} N \\ N \\ CH_2 - CH_2 - O \end{array}$$

RN 199114-47-1 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-48-2 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-51-7 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-.alpha.-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{OH}_2-\text{CH}_2-\text{O} \\ \text{N} & \text{O} & \text{CH}_2-\text{CH}-\text{CO}_2\text{H} \\ \end{array}$$

RN 199114-52-8 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-.alpha.-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

N N
$$\sim$$
 CH₂ - CH₂ - O OH O OH₂ - CH₂ - CH-C- OEt

RN 199114-54-0 CAPLUS

CN Benzaldehyde, 4-[2-(2,5,6-trimethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-55-1 CAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

RN 199114-56-2 CAPLUS

CN 4(3H)-Quinazolinone, 3-[2-(4-aminophenoxy)ethyl]-2-methyl- (9CI) (CA INDEX NAME)

RN 199114-57-3 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-methyl-4-oxo-3(4H)-quinazolinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-59-5 CAPLUS

Benzaldehyde, 4-[2-[2-ethyl-6-oxo-4-(trifluoromethyl)-1(6H)-CN pyrimidinyl]ethoxy]- (9CI) (CA INDEX NAME)

RE.CNT 34

RE

- (3) Anon; 1980, 17, CAPLUS
- (8) Cantello; Journal of Medicinal Chemistry 1994, V37(23), P3977 CAPLUS
- (9) Clark; US 5036079 1991 CAPLUS
- (11) Clark, D; J Med Chem 1991, V34, P319 CAPLUS
- (14) Dow; US 5498621 1996 CAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 2

L81 ANSWER 2 OF 40 CAPLUS COPYRIGHT 2000 ACS

Ι

AN 1999:673737 CAPLUS

DN 132:35672

TI Synthesis and biological activity of some 2-substituted quinazolin-4-ones

AU Spirkova, K.; Stankovsky, S.; Mrvova, A.; Cipak, L'.

CS Department of Organic Chemistry, Faculty of Chemical Technology, Slovak University of Technology, Bratislava, SK-812 37, Slovakia

SO Chem. Pap. (1999), 53(4), 272-275

CODEN: CHPAEG; ISSN: 0366-6352

PB Slovak Academic Press Ltd.

DT Journal

LA English

OS CASREACT 132:35672

GI

ΙR

$$\bigcup_{N} \bigcup_{H} \bigcup_{N} \bigcup_{O}$$

AB The nonclassical antifolates, e.g. 2-morpholinomethyl-3H-quinazolin-4-one (I), have been prepd. by nucleophilic substitution of bromine in

2-bromomethyl-3H-quinazolin-4-one by nitrogen and oxygen nucleophiles.

and 1H NMR spectra, 13C NMR data of selected compds., basic antibacterial and cytotoxic activities are presented.

IT 120244-31-7P 252570-63-1P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and biol. activity of quinazolinones as antibacterial and antitumor agents)

RN 120244-31-7 CAPLUS

CN 4(1H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$\bigcap_{N}^{H} \operatorname{CH}_2 - O \longrightarrow \operatorname{NO}_2$$

RN 252570-63-1 CAPLUS

CN 4(1H)-Quinazolinone, 2-[(2-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} H \\ N \\ O \end{array} - CH_2 - O - \begin{array}{c} O_2N \\ O \end{array}$$

RE.CNT 10

RE

(1) Gupta, C; J Med Chem 1968, V11, P392 CAPLUS

(2) Horakova, K; Neoplasma 1988, V35, P169 CAPLUS
(3) Hudecova, D; Folia Microbiol 1996, V41, P473 CAPLUS

(4) Jantova, S; Cell Biochem Funct 1993, V11, P131 CAPLUS (5) Jantova, S; Folia Microbiol 1997, V42, P324 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/535387 QAZI Page 13

=> d bib abs hitstr 3

```
ANSWER 3 OF 40 CAPLUS COPYRIGHT 2000 ACS
     1999:212642 CAPLUS
AN
     130:223293
DN
     Heterocyclic compounds, process for their preparation and pharmaceutical
TΙ
     compositions containing them and their use in the treatment of diabetes
     and related diseases
     Lohray, Vidya Bhushan; Lohray, Braj Bhushan; Paraselli, Rao Bheema
ΙN
     Reddy's Research Foundation, India; Reddy-Cheminor, Inc.
PΑ
     U.S., 26 pp.
SO
     CODEN: USXXAM
     Patent
DT
     English
LA
FAN.CNT 3
     PATENT NO.
                 KIND DATE
                                         APPLICATION NO. DATE
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                                           -----
                           19990323
    US 5885997
                      A
                                          US 1996-777627 19961231
PΙ
     CA 2258949
                     AA ,19971106
A2 19971106
                                          CA 1997-2258949 19970630
                                     WO 1997-US11522 19970630
     WO 9741097
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ,
             VN, YU, ZW
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     AU 9737198
                     A1 19971119
                                          AU 1997-37198
                                                            19970630
     US 5985884
                      Α
                            19991116
                                          US 1997-884816
                                                            19970630
     NO 9806055
                      Α
                            19981222
                                          NO 1998-6055
                                                            19981222
PRAI IN 1996-DE1150
                      19960701
     US 1996-777627
                      19961231
     WO 1997-US11522 19970630
     MARPAT 130:223293
GΙ
```

AΒ The present invention relates to novel antidiabetic compds., their tautomeric forms, their derivs., their stereoisomers, their polymorphs, their pharmaceutically acceptable salts, their pharmaceutically acceptable

solvates and pharmaceutically acceptable compns. contq. them. This invention particularly relates to novel azolidinedione derivs., and their pharmaceutically acceptable salts, pharmaceutically acceptable solvates and pharmaceutical compns. contg. them. Approx. 30 title compds. such as I (R = Pr, Me, Et, Bu, benzyl) and their quinazoline analogs were prepd. in 66-99% yields, e.g., by condensation of aldehydes II with thiazolidine-2,4-dione. Antidiabetic data was given for several of the prepd. compds. At 30 mg/kg/day, after 6 days,

5-[4-[2-[2-ethyl-4-methyl-6-

oxo-1,5-dihydro-1-pyrimidinyl]ethoxy]phenylmethyl] thiazolidine-2,4-dione reduced the blood glucose level 73%, lowered triglycerides 70% and also lowered cholesterol in the rat.

IΤ 199114-24-4P 199114-25-5P 199114-26-6P 199114-27-7P 199114-28-8P 199114-29-9P 199114-30-2P 199114-31-3P 199114-32-4P 199114-33-5P 199114-34-6P 199114-35-7P 199114-36-8P 199114-37-9P 199114-38-0P 199114-39-1P 199114-40-4P 199114-41-5P 199114-42-6P 199114-43-7P 199114-44-8P 199114-45-9P 199114-46-0P 199114-47-1P

199114-48-2P 199114-51-7P 199114-52-8P

199114-54-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of pyrimidinylethoxybenzylthiazolidinediones)

RN 199114-24-4 CAPLUS

Benzaldehyde, 4-[2-(4-methyl-6-oxo-2-propyl-1(6H)-pyrimidinyl)ethoxy]-CN (9CI) (CA INDEX NAME)

199114-25-5 CAPLUS RN Benzaldehyde, 4-[2-(2,4-dimethyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]- (9CI) (CA INDEX NAME)

199114-26-6 CAPLUS RN Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \\ \text{N} & \text{N--} \text{CH}_2\text{--} \text{CH}_2\text{--} \text{O} \\ \\ \text{Me} & \text{O} & \text{CHO} \end{array}$$

199114-27-7 CAPLUS RN Benzaldehyde, 4-[2-(2-butyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-CN (9CI) (CA INDEX NAME)

199114-28-8 CAPLUS RN CN Benzaldehyde, 4-[2-[4-methyl-6-oxo-2-(phenylmethyl)-1(6H)pyrimidinyl]ethoxy]- (9CI) (CA INDEX NAME)

Ph CH₂
N N-CH₂-CH₂-O
CHO

RN 199114-29-9 CAPLUS

CN Benzaldehyde, 4-[2-(2,5-diethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

Me CH₂ CH₂ O CHO

RN 199114-30-2 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-6-oxo-4-phenyl-1(6H)-pyrimidinyl)ethoxy](9CI) (CA INDEX NAME)

RN 199114-31-3 CAPLUS

CN Acetamide, N-[1-[2-(4-formylphenoxy)ethyl]-1,2-dihydro-2-oxo-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

N — CH2 — CH2 — O — CHO

RN 199114-32-4 CAPLUS

CN Benzaldehyde, 4-[2-(4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-33-5 CAPLUS

CN Benzaldehyde, 4-[2-(2-methyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-34-6 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-35-7 CAPLUS

CN Benzaldehyde,

4-[2-(2-methyl-4-oxopyrido[2,3-d]pyrimidin-3(4H)-yl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-36-8 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy](9CI) (CA INDEX NAME)

RN 199114-37-9 CAPLUS

CN Benzaldehyde, 4-[(3-ethyl-3,4-dihydro-4-oxo-2-quinazolinyl)methoxy]-(9CI)

(CA INDEX NAME)

RN 199114-38-0 CAPLUS

CN Benzaldehyde, 4-[(1,4-dihydro-1-methyl-4-oxo-2-quinazolinyl)methoxy]- (9CI) (CA INDEX NAME)

RN 199114-39-1 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]-3-methoxy- (9CI) (CA INDEX NAME)

Searched by John Dantzma

703-308-4488

RN 199114-40-4 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, 1-oxime (9CI) (CA INDEX NAME)

N N
$$CH_2$$
 CH_2 O CH N O

RN 199114-41-5 CAPLUS

CN 4(3H)-Pyrimidinone,

2-ethyl-3-[2-[4-[(hydroxyamino)methyl]phenoxy]ethyl]-6methyl- (9CI) (CA INDEX NAME)

RN 199114-42-6 CAPLUS

CN Urea,

N-[[4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]phenyl]methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 199114-43-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-ethyl-6-methyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

RN 199114-44-8 CAPLUS

CN 4(3H) -Quinazolinone, 2-ethyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX

Searched by John Dantzma 703-308-4488

NAME)

RN 199114-45-9 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl-6-methyl- (9CI) (CA INDEX NAME) *

$$\begin{array}{c|c} \text{Et} & \\ \text{N} & \text{N--} \text{CH}_2\text{--} \text{CH}_2\text{--} \text{O} \\ \\ \text{Me} & \text{O} & \text{NH}_2 \end{array}$$

RN 199114-46-0 CAPLUS

CN 4(3H)-Quinazolinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl- (9CI) (CA INDEX

NAME)

RN 199114-47-1 CAPLUS

CN Benzenepropanoic acid, *.alpha.-bromo-4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-48-2 CAPLUS

CN Benzenepropanoic acid, .alpha.~bromo-4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-51-7 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-.alpha.-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{N---} \\ \text{CH}_2 - \text{CH}_2 - \text{O} \\ \text{OH} \\ \text{CH}_2 - \text{CH} - \text{CO}_2 \\ \text{H} \end{array}$$

RN 199114-52-8 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)+pyrimidinyl)ethoxy]-.alpha.-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-54-0 CAPLUS

CN Benzaldehyde, 4-[2-(2,5,6-trimethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethoxy]- (9CI) (CA INDEX NAME)

RE.CNT 57

RE

- (1) Anon; EP 008203 A 1980 CAPLUS
- (6) Anon; EP 0207581 1987 CAPLUS
- (8) Anon; EP 0306228 1989 CAPLUS
- (9) Anon; EP 0332331 1989 CAPLUS
- (10) Anon; EP 0332332 1989 CAPLUS

Searched by John Dantzma

703-308-4488

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 4

```
ANSWER 4 OF 40 CAPLUS COPYRIGHT 2000 ACS
L81
ΑN
      1999:152363 CAPLUS
DN
      130:196665
ΤI
      Preparation of .omega.-[(oxoquinazolinylalkoxy)phenyl]alkanoates and
      analogs as PPAR.alpha. and PPAR.gamma. receptor agonists
IN
      Lohray, Vidya Hushan; Lohray, Braj Bhushan; Paraselli, Rao Bheema;
      Ramanujam, Rajagopalan; Chakrabarti, Ranjan
      Reddy's Research Foundation, India; Reddy-Cheminor, Inc.
PΑ
      PCT Int. Appl., 140 pp.
SO
      CODEN: PIXXD2
DT
      Patent
LA
     English
FAN.CNT 1
      PATENT NO.
                    KIND DATE
                                                 APPLICATION NO. DATE
                               ----
                                                 -----
     WO 9908501
                         A2
PΙ
                                19990225
                                                 WO 1998-US22568 19981026
     WO 9908501
                         АЗ
                                19990415
               AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK,
               EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO,
               NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
               CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI US 1998-82825
                         19980423
     MARPAT 130:196665
GΙ
```

$$R^{1}$$
 R^{2}
 R^{3}
 R^{3}

AB Title compds. [I; R = (CH2)nOZCHR4CR5(OR6)COYR7 and R3 = H, halo, alkyl, alkoxy, etc.; R = H, OH, acyl, alkyl, etc.; and R3 = (CH2)nOZCHR4CR5(OR6)COYR7; R1,R2 = H, halo, alkyl, alkoxy, etc.; R1R2 = atoms to complete a ring; R4,R5 = H, halo, alkyl, alkoxy, etc.;; R4R5 = bond; R6 = H, acyl, alkyl aryl, etc.; R7 = H, alkyl, heterocyclyl, (hetero)aryl, etc.; X = O or S; Y = O or NR8; R8 = H, alkyl, aryl, etc.; R7R8 = atoms to complete a ring; Z = (hetero)arylene; n = 1-4] were prepd.

Thus, I (R = Me, R1R2 = CH:CHCH:CH, X = O)(II; R3 = CH2C1) was condensed with 4-(HO)C6H4CH2CH(OEt)CO2Et to give II [R3 = CH2OC6H4[CH2CH(OEt)CO2Et]-

4]. Data for biol. activity of I were given.

IT 220746-26-9P 220746-27-0P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic Searched by John Dantzma 703-308-4488

preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); USES (Uses)

(prepn. of .omega.~[(oxoquinazolinylalkoxy)phenyl]alkanoates and analogs as PPAR.alpha. and PPAR.gamma. receptor agonists)

RN 220746-26-9 CAPLUS

CN Benzenepropanoic acid, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]-.alpha.-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

RN 220746-27-0 CAPLUS

CN Benzenepropanoic acid, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]-.alpha.-hydroxy- (9CI) (CA INDEX NAME)

=> d bib abs hitstr 5

```
ANSWER 5 OF 40 CAPLUS, COPYRIGHT 2000 ACS
     1999:64689 CAPLUS
DN
     130:139576
     Preparation of cyclin dependent kinase inhibiting purine derivatives
TI
     Griffin, Roger John; Calvert, Alan Hilary; Curtin, Nicola Jane; Newell,
     David Richard; Golding, Bernhard Thomas; Endicott, Jane Anne; Noble,
     Martin Edward Mantyla; Boyle, Francis Thomas; Jewsbury, Philip John
PΑ
     Newcastle University Ventures Limited, UK
SO
     PCT Int. Appl., 92 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO. DATE
PΙ
     WO 9902162
                            19990121
                      A1
                                           WO 1998-GB2025
                                                            19980710
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG,
             KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX,
             NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
             UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     AU 9882342
                      Α1
                            19990208
                                         AU 1998-82342
                                                            19980710
PRAI GB 1997-14603
                      19970712
     GB 1998-6743
                      19980328
                      19980710
     WO 1998-GB2025
OS
    MARPAT 130:139576
GΙ
```

Purine derivs. I [X = O, S or CHRx; Rx = H, C1-4-alkyl; D = H, halo, NZ1Z2; Z1, Z2 = H, C1-4-alkyl, C1-4-hydroxyalkyl; A = H, C1-4-alkyl, C1-4-alkoxy, OH, CH2(CH2)nOH, NRalRa2; n = 1 - 4; Ra1, Ra2 = H, C1-4-alkyl; B = H, C1-4-alkyl, C1-4-alkoxy, CF3, (un)substituted aryl, (e.g. Ph), (un)substituted aralkyl (e.g. benzyl), hydroxy group that provides a C=O tautomer; Y = (un)substituted C4-8-carbocyclic, -heterocyclic ring, (un)substituted linear or branched hydrocarbon chain) which can act as inhibitors of cyclin dependent kinases (CDKs) and which thereby can provide useful therapeutic compds. for use in treatment of Searched by John Dantzma 703-308-4488

tumors or other cell proliferation disorders are disclosed. The compds. of this invention bind to CDK mols. in a manner that appears to be different to that of known CDK inhibitors such as olomoucine and roscovitine. Thus, O6-[(cyclohex-3-en-1-yl)methyl]guanine (II) was

from 2-amino-6-chloropurine via addn. to 3-cyclohexenemethanol in THF contg. sodium hydride. II is an active inhibitor of cyclin dependent kinases: IC50 = 3.2 .mu.M vs. CDK1, 87% inhibition of CDK2 at 100.mu.M

and

53% inhibition of CDK4.

219991-62-5P, 2-Amino-6-[(uracil-5-yl)methoxy]-8-oxopurine ITRL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of purine derivs. as cyclin dependent kinase inhibitors)

RN 219991-62-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-[[(2-amino-7,8-dihydro-8-oxo-1H-purin-6yl)oxy]methyl]- (9CI) (CA INDEX NAME)

RE.CNT 15

(1) Arris, C; Anti-Cancer Drug Design 1994, V9(5), P401 CAPLUS

(5) Chae, M; Journal of Medicinal Chemistry 1994, V37(3), P342 CAPLUS(6) Chae, M; Journal of Medicinal Chemistry 1995, V38(2), P359 CAPLUS

(8) Havlicek, L; Journal of Medicinal Chemistry 1997, V40(4), P408 CAPLUS (10) Krenitsky, T; Journal of Medicinal Chemistry 1989, V32(7), P1471 CAPLUS

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d bib abs hitstr 6

L81 ANSWER 6 OF 40 CAPLUS COPYRIGHT 2000 ACS 1998:485432 CAPLUS ΑN 129:175649 DN ΤI Quinazolines useful as nitric oxide synthase (NOS) inhibitors ΙN Gaku, Kazuhiko; Nishino, Shigetaka; Fuji, Tetsuo; Kato, Takeshi PΑ Fujisawa Pharmaceutical Co., Ltd., Japan Jpn. Kokai Tokkyo Koho, 16 pp. SO CODEN: JKXXAF DTPatent LA Japanese FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ---------_____ PΙ JP 10195058 A2 19980728 JP 1997-352820 19971222 PRAI AU 1996-4404 19961230

MARPAT 129:175649

OS

GΙ

Quinazolines I [R1 = H, halo, substituted lower alkylamino; R2, R3 = H, halo; R4 = H, amino, acylamino, di(lower)alkylamino, amidino, thiazolinylamino, [(imino)(thienyl)methyl]amino, piperidino, 1-imidazolvl,

cyano, OH, acyloxy, protected carboxy, dioxolanyl, oxotetrahydropyranyl, (imino) (lower alkoxy) methyl; A1 = lower alkylene; A2 = bond, O, NH, CHOH, CO; A3 = bond, phenylene, pyridonediyl, (lower alkoxy-substituted) pyridinediyl; A4 = bond, lower alkylene; when A2 is CO, then A4 is lower alkylene; when both A2 and A3 are bonds, then R4 is not H nor protected carboxy] or their salts, useful as NOS inhibitors for treatment of various

diseases, are claimed. Biol. activity data are not given. Cyclization of

N-[2-[2-[(2-carbamoyl-3,5-dichlorophenyl)amino]ethoxy]benzyl]acetam ide (prepn. given) with 0.18 g 1,1'-carbonyldiimidazole gave 0.13 g N-[2-[2-(5,7-dichloro-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-1yl)ethoxy]benzyl]acetamide.

IT211378-78-8P

> RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of quinazolines as nitric oxide synthase inhibitors)

211378-78-8 CAPLUS RN

> Searched by John Dantzma 703-308-4488

2,4(1H,3H)-Quinazolinedione, 1-[2-(2-aminophenoxy)ethyl]-5,7-dichloro-, monohydrochloride (9CI) (CA INDEX NAME)CN

HCl

=> d bib abs hitstr 7

```
ANSWER 7 OF 40 CAPLUS COPYRIGHT 2000 ACS
     1997:740205 CAPLUS
DN
     128:13282
     Preparation of thiazolidinediones and analogs as antidiabetics
TI
     Lohray, Vidya Bhushan; Lohray, Braj Bhushan; Paraselli, Rao Bheema;
     Gurram, Ranga Madhavan; Ramanujam, Rajagopalan; Chakrabarti, Ranjan;
     Pakala, Sarma K. S.
     Dr. Reddy's Research Foundation, India; Reddy-Cheminor, Inc.
PA
     PCT Int. Appl., 112 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 3
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO. DATE
PΙ
     WO 9741097
                            19971106
                      Α2
                                           WO 1997-US11522 19970630
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ,
             VN, YU, ZW
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     US 5885997
                            19990323
                       Α
                                           US 1996-777627
                                                            19961231
     AU 9737198
                       Α1
                            19971119
                                           AU 1997-37198
                                                            19970630
     EP 958296
                       Α1
                            19991124
                                           EP 1997-934041
                                                            19970630
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE, PT, IE, FI
     NO 9806055
                            19981222
                                         NO 1998-6055
                      Α
                                                            19981222
PRAI US 1996-777627
                      19961231
     IN 1996-DE1150
                      19960701
     WO 1997-US11522 19970630
OS
     MARPAT 128:13282
GΙ
```

AB Title compds. [I; A = N, CR5; B = O or S; R = CHR4ZO(CH2)nR1; R1 = (un)substituted pyrimidinyl, -quinazolinyl, etc.; R4,R5 = H, halo, alkyl; R4R5 = bond; Z = divalent arom. or heterocyclic group; n = 1-4] were prepd. Thus, 4-methyl-2-propyl-1,6-dihydro-6-pyrimidinone was N-alkylated

by 4-(BrCH2CH2O)C6H4CHO and the product condensed with Searched by John Dantzma 703-308-4488 thiazolidine-2,4-dione to give, after hydrogenation, title compd. II. Data for biol. activity of I were given.

IT 199114-24-4P 199114-25-5P 199114-26-6P

199114-27-7P 199114-28-8P 199114-29-9P

199114-30-2P 199114-31-3P 199114-32-4P

199114-33-5P 199114-34-6P 199114-35-7P

199114-36-8P 199114-37-9P 199114-38-0P

199114-39-1P 199114-40-4P 199114-41-5P

199114-42-6P 199114-43-7P 199114-44-8P

199114-45-9P 199114-46-0P 199114-47-1P

199114-48-2P 199114-51-7P 199114-52-8P

199114-54-0P 199114-55-1P 199114-56-2P

199114-57-3P 199114-59-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of thiazolidinediones and analogs as antidiabetics)

RN 199114-24-4 CAPLUS

CN Benzaldehyde, 4-[2-(4-methyl-6-oxo-2-propyl-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-25-5 CAPLUS

CN Benzaldehyde, 4-[2-(2,4-dimethyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]- (9CI) (CA INDEX NAME)

Me N
$$\sim$$
 CH₂ CH₂ \sim CHC CHC

RN 199114-26-6 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-27-7 CAPLUS

CN Benzaldehyde, 4-[2-(2-butyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]- (9CI) (CA INDEX NAME)

Searched by John Dantzma 703-308-4488

$$\begin{array}{c|c} & \text{N-Bu} \\ & \text{N} & \text{N-CH}_2\text{-CH}_2\text{-O-} \\ & \text{Me} & \text{O} & \text{CHO} \end{array}$$

RN 199114-28-8 CAPLUS

CN Benzaldehyde, 4-[2-[4-methyl-6-oxo-2-(phenylmethyl)-1(6H)-6-oxo-2-(phenylmethyl)]pyrimidinyl]ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-29-9 CAPLUS

Benzaldehyde, 4-[2-(2,5-diethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-CN (9CI) (CA INDEX NAME)

Me
$$N$$
 N CH_2 CH_2 O CH_2

RN 199114-30-2 CAPLUS

CNBenzaldehyde, 4-[2-(2-ethyl-6-oxo-4-phenyl-1(6H)-pyrimidinyl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-31-3 CAPLUS

CN Acetamide, N-[1-[2-(4-formylphenoxy)ethyl]-1,2-dihydro-2-oxo-4pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 199114-32-4 CAPLUS

Benzaldehyde, 4-[2-(4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX CN

RN 199114-33-5 CAPLUS

CN Benzaldehyde, 4-[2-(2-methyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA INDEX NAME)

RN 199114-34-6 CAPLUS

Benzaldehyde, 4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]- (9CI) (CA CN INDEX NAME)

RN 199114-35-7 CAPLUS

CN Benzaldehyde,

4-[2-(2-methyl-4-oxopyrido[2,3-d]pyrimidin-3(4H)-yl)ethoxy]-(9CI) (CA INDEX NAME)

RN 199114-36-8 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]- (9CI) (CA INDEX NAME)*

RN 199114-37-9 CAPLUS

CN Benzaldehyde, 4-[(3-ethyl-3,4-dihydro-4-oxo-2-quinazolinyl)methoxy]-(9CI)

(CA INDEX NAME)

RN 199114-38-0 CAPLUS

CN Benzaldehyde, 4-[(1,4-dihydro-1-methyl-4-oxo-2-quinazolinyl)methoxy](9CI) (CA INDEX NAME)

RN 199114-39-1 CAPLUS

CN Benzaldehyde, 4-[(3,4-dihydro-3-methyl-4-oxo-2-quinazolinyl)methoxy]-3-Searched by John Dantzma 703-308-4488 methoxy- (9CI) (CA INDEX NAME)

RN 199114-40-4 CAPLUS

CN Benzaldehyde, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, 1-oxime (9CI) (CA INDEX NAME)

RN 199114-41-5 CAPLUS

CN 4(3H)-Pyrimidinone,

2-ethyl-3-[2-[4-[(hydroxyamino)methyl]phenoxy]ethyl]-6methyl- (9CI) (CA INDEX NAME)

N N
$$\sim$$
 CH₂ \sim CH₂ \sim CH₂ \sim NH \sim OH

RN 199114-42-6 CAPLUS

CN Urea,

 $\begin{tabular}{ll} N-[[4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]phenyl]methyl]-N-hydroxy- (9CI) (CA INDEX NAME) \\ \end{tabular}$

RN 199114-43-7 CAPLUS

CN 4(3H)-Pyrimidinone, 2-ethyl-6-methyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

Searched by John Dantzma 703-308-4488

N N
$$\sim$$
 CH₂-CH₂-O \sim NO₂

RN 199114-44-8 CAPLUS

CN 4(3H)-Quinazolinone, 2-ethyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX

NAME)

RN 199114-45-9 CAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl-6-methyl- (9CI) (CA INDEX NAME)

N
$$\sim$$
 CH $_2$ CH $_2$ O \sim NH $_2$

RN 199114-46-0 CAPLUS

CN 4(3H)-Quinazolinone, 3-[2-(4-aminophenoxy)ethyl]-2-ethyl- (9CI) (CA INDEX

NAME)

RN 199114-47-1 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

703-308-4488

RN 199114-48-2 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-ethyl-4-oxo-3(4H)-quinazolinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 199114-51-7 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-.alpha.-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{N---} \text{CH}_2\text{---} \text{CH}_2\text{---} \text{O} \\ \\ \text{Me} \\ \end{array} \begin{array}{c} \text{OH} \\ \\ \text{CH}_2\text{---} \text{CH---} \text{CO}_2\text{H} \\ \end{array}$$

RN 199114-52-8 CAPLUS

CN Benzenepropanoic acid, 4-[2-(2-ethyl-4-methyl-6-oxo-1(6H)-pyrimidinyl)ethoxy]-.alpha.-hydroxy-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{N-} \\ \text{CH}_2 - \text{CH}_2 - \text{O} \\ \text{OH} \\ \text{O} \\ \end{array} \begin{array}{c} \text{OH} \\ \text{O} \\ \text{CH}_2 - \text{CH-} \\ \text{C-} \\ \text{OEt} \\ \end{array}$$

RN 199114-54-0 CAPLUS

CN Benzaldehyde, 4-[2-(2,5,6-trimethyl-4-oxothieno[2,3-d]pyrimidin-3(4H)-yl)ethoxy]- (9CI) (CA*INDEX NAME)

OHC O Me Me Me

RN 199114-55-1 CAPLUS

CN 4(3H)-Quinazolinone, 2-methyl-3-[2-(4-nitrophenoxy)ethyl]- (9CI) (CA INDEX NAME)

 $\begin{array}{c} N \\ N \\ O \end{array}$

RN 199114-56-2 CAPLUS

CN 4(3H)-Quinazolinone, 3-[2-(4-aminophenoxy)ethyl]-2-methyl- (9CI) (CA INDEX NAME)

N Me NH₂ CH₂ - CH₂ - O NH₂

RN 199114-57-3 CAPLUS

CN Benzenepropanoic acid, .alpha.-bromo-4-[2-(2-methyl-4-oxo-3(4H)-quinazolinyl)ethoxy]-, ethyl ester (9CI) (CA INDEX NAME)

Me CH2-CH2-O-CH2-O-CH2-CH-C-OEt

RN 199114-59-5 CAPLUS

CN Benzaldehyde, 4-[2-[2-ethyl-6-oxo-4-(trifluoromethyl)-1(6H)-pyrimidinyl]ethoxy]- (9CI) (CA INDEX NAME)

$$N$$
 N
 N
 CH_2
 CH_2
 CH_2
 CH_3
 CH_3

Searched by John Dantzma 703-308-4488

CN 1167764

MARPAT 127:205585

PRAI JP 1996-14898

GI

ANSWER 8 OF 40 CAPLUS COPYRIGHT 2000 ACS ΑN 1997:553183 CAPLUS DN 127:205585 TIPreparation of benzoazines for reducing blood glucose level ΙN Nagao, Yoshihiro; Ito, Yoshikuni; Kotake, Jiro; Kouda, Tadayuki; Honda, Haruyoshi; Sato, Susumu; Matsuda, Hideaki PΑ SS Pharmaceutical Co., Ltd., Japan SO Eur. Pat. Appl., 21 pp. CODEN: EPXXDW DT Patent LA English FAN.CNT 1 PATENT NO. KIND * DATE APPLICATION NO. -----------EP 787727 PΙ A1 19970806 EP 1997-101626 19970131 R: BE, CH, DE, ES, FR, GB, IT, LI, NL, SE JP 09268189 A2 19971014 JP 1997-15135 19970129 CA 2196400 AA19970801 CA 1997-2196400 19970130 US 5710152 Α 19980120 US 1997-791269 19970130

CN 1997-101300

19970131

$$\begin{bmatrix} R^1 & & & & \\ & &$$

Α

19960131

19971217

AB The title compds. [I; R1 = alkyl, alkoxy, halo, etc.; R2, R3 = H, alkyl; R2R3 = C2-7 alkylene; R4, R5 = H, alkyl; X = O, S, NR6 (wherein R6 = H, alkyl, aryl, pyridyl); m = 0-4; n = 1-3] which exhibit superior effects for reducing blood glucose value, plasma insulin value, and plasma triglyceride value, and are useful as a medicament for preventing or treating diabetes, hyperlipidemia, and obesity, were prepd. Thus, reaction of 4-[2-(4-oxo-3,4-dihydro-2H-1,3-benzoxazin-3-yl)ethoxy]benzaldehyde with 2,4-thiazolidinedione in the presence of a Searched by John Dantzma 703-308-4488

catalytic amt. of AcOH and piperidine in PhMe followed by hydrogenation

- of the resulting thiazolidinedione II over 10% Pd/C in 1,4~dioxane afforded
- [R1-R5 = H; X = O; n = 1] which showed 65.8% blood glucose redn. at 9.8 mg/kg/day.
- IT 194713-69-4P 194713-70-7P 194713-71-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of benzoazines for reducing blood glucose level)

- RN 194713-69-4 CAPLUS
- CN Benzaldehyde,
- 4-[2-(1,4-dihydro-4-oxo-1-phenyl-3(2H)-quinazolinyl)ethoxy]-(9CI) (CA INDEX NAME)

- RN 194713-70-7 CAPLUS
- CN Benzaldehyde,
- 4-[2-(1,4-dihydro-1-methyl-4-oxo-3(2H)-quinazolinyl)ethoxy]-(9CI) (CA INDEX NAME)

- RN 194713-71-8 CAPLUS
- CN Benzaldehyde, 4-[2-[1,4-dihydro-4-oxo-1-(2-pyridinyl)-3(2H)-quinazolinyl]ethoxy]- (9CI) (CA INDEX NAME)

QAZI 09/535387 Page 42

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=> d bib abs hitstr 9
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ANSWER 9 OF 40 CAPLUS COPYRIGHT 2000 ACS
L81
         1995:887878 CAPLUS
ΑN
         123:286023
 DN
TI
         Preparation of 5-[4-(heterocyclylalkoxy)benzyl - or
         benzylidene]thiazolidine-2,4-dione derivatives as hypolipidemics and
         hypoglycemics
 IN
         Yano, Shingo; Ogawa, Kazuo; Fukushima, Masakazu
 PΑ
         Taiho Pharmaceutical Co Ltd, Japan
         Jpn. Kokai Tokkyo Koho, 57 pp.
SO
         CODEN: JKXXAF
DT
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         Japanese
LA
FAN.CNT 1
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                                      KIND DATE
                                                                             APPLICATION NO. DATE
         -----
                                        ----
                                                                               -----
                                         A2
         JP 07138258
                                                    19950530
PI
                                                                             JP 1993-286509
                                                                                                               19931116
         CA 2177553
                                        AA
                                                    19971129
                                                                              CA 1996-2177553 19960528
PRAI JP 1993-286509 19931116
         MARPAT 123:286023
GΙ
         For diagram(s), see printed CA Issue.
         The title compds. [I; R1, R2 = H, halo, lower (halo)alkyl or
(halo)alkoxy;
         or R1 and R2 are bonded together to form C1-3 alkylenedioxy; X = N, CH;
         the single bond with a dotted line represents a single bond or a double
         bond; A = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, lower alkyl; n = heterocyclyl selected from Q - Q5; R3, R4 = H, low
         1-4], having little side effects and useful as antidiabetics having
         activity for lowering both sugar and lipids in blood, are prepd. Thus, a
         soln. of benzaldehyde deriv. Q6-CHO (R1 = CF3) (prepn. given) 9.5,
         2,4-thiazolidinone 3.8, and AcONa 4.3 g in 50 mL toluene was refluxed for
         15 h and the solvent was removed by distn. to give, after treatment with
         80% aq. AcOH and filtration of pptd. crystals, 76% 5-benzylidene-2,4-
         thiazolidinone deriv. (II; R = Q6, wherein R1 = CF3) which was
         hydrogenated over 5% Pd-C in 1,4-dioxane at 50.degree. and H pressure 50
         atm to give 80% 5-benzyl-2,4-thiazolidinone deriv. (III; R = \sqrt{26}, wherein
         R1 = CF3) (IV). IV and III (R = Q6, wherein R1 = CF30) at 2.5 mg/kg p.o.
         twice a day for 5 consecutive days lowered the blood sugar level by 41
and
         53%, resp., in mice.
         169548-02-1P 169548-03-2P 169548-04-3P
         169548-05-4P 169548-06-5P 169548-07-6P
         169548-08-7P 169548-09-8P 169548-10-1P
         169548-11-2P 169548-12-3P 169548-13-4P
         169548-14-5P 169548-15-6P 169548-16-7P
         169548-17-8P 169548-18-9P 169548-19-0P
         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
               (intermediate for prepn. of [(heterocyclylalkoxy)benzyl - or
               benzylidene]thiazolidinedione derivs. as hypolipidemics and
               hypoglycemics)
RN
         169548-02-1 CAPLUS
CN
         Benzaldehyde, 4-[2-[2-oxo-3-[4-(trifluoromethoxy)phenyl]-1-
```

imidazolidinyl]ethoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN

169548-03-2 CAPLUS Benzaldehyde, 4-[2-[2-0x0-3-[4-(trifluoromethyl)phenyl]-1-imidazolidinyl]ethoxy]- (9CI) (CA INDEX NAME) CN

PAGE 1-A

PAGE 2-A

CF3

169548-04-3 CAPLUS RN

CN

Benzaldehyde, 4-[2-[3-(4-chlorophenyl)-2-oxo-1-imidazolidinyl]ethoxy]-(9CI) (CA INDEX NAME)

169548-05-4 CAPLUS CN Benzaldehyde, 4-[2-[3-(3,4-difluorophenyl)-2-oxo-1-imidazolidinyl]ethoxy]-(9CI) (CA INDEX NAME)

RN 169548~06-5 CAPLUS

CN Benzaldehyde,

4-[2-[3-(2,4-dichlorophenyl)-2-oxo-1-imidazolidinyl]ethoxy]-(9CI) (CA INDEX NAME)

169548-07-6 CAPLUS RN

Benzaldehyde, 4-[2-[3-(1,3-benzodioxol-5-yl)-2-oxo-1-CN imidazolidinyl]ethoxy]- (9CI) (CA INDEX NAME)

RN 169548-08-7 CAPLUS

Benzaldehyde, 4-[2-(2-oxo-3-phenyl-1-imidazolidinyl)ethoxy]- (9CI) (CA CN INDEX NAME)

CH₂

CH₂

169548-09-8 CAPLUS RN

Benzaldehyde, 4-[2-[3-(4-chloro-2-fluorophenyl)-2-oxo-1-CN imidazolidinyl]ethoxy]- (9CI) (CA INDEX NAME)

RN 169548-10-1 CAPLUS

Benzaldehyde, 4-[2-[3-(4-methoxyphenyl)-2-oxo-1-imidazolidinyl]ethoxy]-CN (9CI) (CA INDEX NAME)

ОМе

CN

RN 169548-11-2 CAPLUS

Benzaldehyde, 4-[2-[3-(4-fluorophenyl)-2-oxo-1-imidazolidinyl]ethoxy]-(9CI) (CA INDEX NAME)

F

RN 169548-12-3 CAPLUS
CN Benzaldehyde, 4-[2-[3-(3-fluorophenyl)-2-oxo-1-imidazolidinyl]ethoxy]Searched by John Dantzma 703-308-4488

(9CI) (CA INDEX NAME)

RN 169548-13-4 CAPLUS
CN Benzaldehyde, 4-[2-[3-(2-methoxyphenyl)-2-oxo-1-imidazolidinyl]ethoxy](9CI) (CA INDEX NAME)

RN 169548-14-5 CAPLUS
CN Benzaldehyde, 4-[2-[2-0x0-3-(3-pyridinyl)-1-imidazolidinyl]ethoxy]- (9CI)
(CA INDEX NAME)

Searched by John Dantzma 703-308-4488

Page 50

QAZI 09/535387

RN 169548-15-6 CAPLUS
CN Benzaldehyde, 4-[2-[3-(6-methoxy-3-pyridinyl)-2-oxo-1-imidazolidinyl]ethoxy]- (9CI) (CA INDEX NAME)

OMe

RN 169548-16-7 CAPLUS
CN Benzaldehyde, 4-[3-[3-(4-chlorophenyl)-2-oxo-1-imidazolidinyl]propoxy]Searched by John Dantzma 703-308-4488

(9CI) (CA INDEX NAME)

169548-17-8 CAPLUS RN Benzaldehyde, 4-[3-[2-oxo-3-[4-(trifluoromethyl)phenyl]-1imidazolidinyl]propoxy] - (9CI) (CA INDEX NAME)

RN 169548-18-9 CAPLUS CN Benzaldehyde, 4-[3-[3-(3,4-difluorophenyl)-2-oxo-1-imidazolidinyl]propoxy]-Searched by John Dantzma 703-308-4488

(9CI) (CA INDEX NAME)

RN 169548-19-0 CAPLUS

CN Benzaldehyde, 4-[3-[3-(4-chloro-2-fluorophenyl)-2-oxo-1-imidazolidinyl]propoxy]- (9CI) (CA INDEX NAME)

IT 169548-93-0

RL: RCT (Reactant)
(reaction in prepn. of [(heterocyclylalkoxy)benzyl - or
Searched by John Dantzma 703-308-4488

QAZI 09/535387

Page 53

benzylidene]thiazolidinedione derivs. as hypolipidemics and

RN

hypoglycemics)

169548-93-0 CAPLUS

Benzaldehyde, 4-[[1-(4-ethylphenyl)-5-methyl-2-oxo-4-imidazolidinyl]methoxy]- (9CI) (CA INDEX NAME) CN

L81 ANSWER 10 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1995:572524 CAPLUS

DN 123:228160

TI Synthesis, activity and toxicity of novel macrocyclic ligands against HIV-1 in Jurkat and CEM-SS cell lines

AU Balogh-Nair, V.; Brathwaite, C. E.; Chen, C. X.; Vargas, J., Jr.

CS Dep. Chem., The City College of New York, New York, NY, 10031, USA

SO Cell. Mol. Biol. (Paris) (1995), 41(Suppl. 1), S9-S14 CODEN: CMOBEF; ISSN: 0145-5680

DT Journal

LA English

AB A synthetic routes that affords metal-free macrocycles contg. different functionalities in their framework was developed. Novel oxaziridine-contg. and amide-contg. macrocycles were synthesized, and the metal complexes of the latter were also prepd. A series of theophylline and thymidine side-arm contg. podands as well as macrocycles were obtained

employing the same methodol. The primary anti-viral tests of these synthetic compds. for anti-HIV activity was carried out using the XTT-based cytotoxicity assay (CEM-SS cells) with AZT as pos. control. It was found that the nature of the macrocyclic headgroups affected the anti-HIV-1 activity. Heteroatom contg. macrocyclic headgroups displayed activity in the micromolar range. Metal complexation did not enhance the activity and side-arm substitution resulted in inactive compds. Cell viability detd. in both Jurkat and CEM-SS cells was strongly dependent on the structure of the macrocyclic framework. The oxaziridine moieties in the macrocycle were highly toxic to CEM-SS and less toxic to Jurkat cell lines, while amide contg. macrocycles were toxic to neither.

IT 168650-19-9P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and virucidal activity and toxicity of macrocyclic ligands)

RN 168650-19-9 CAPLUS

CN 1H-Purine-2,6-dione, 7,7'-[methylenebis[(4-nitro-2,1-phenylene)oxy-2,1-ethanediyl]]bis[3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

Me N
$$\sim$$
 CH₂ \sim CH₂ \sim CH₂ \sim NO₂ N \sim NO

- L81 ANSWER 11 OF 40 CAPLUS COPYRIGHT 2000 ACS
- AN 1995:560596 CAPLUS
- DN 122:309889
- TI Potential bioreductively activated hypoxia probes and post-irradiation radiosensitizers related to NITP
- AU Mehta, Lina K.; Monney, Hugh; Parrick, John; Hodgkiss, Richard J.
- CS Chem. Dep., Brunel Univ., Middlesex, UB8 3PH, UK
- SO Anti-Cancer Drug Des. (1995), 10(3), 227-41 CODEN: ACDDEA; ISSN: 0266-9536
- DT Journal
- LA English
- AB NITP (1) is an effective marker of hypoxia in tumors for both microscopy and cell sorting studies and, addnl., the compd. shows postirradn. sensitization, probably by inhibition of repair of radiation damage to DNA. However, NITP does not have the substitution pattern which the immunochem. reagents are raised to recognize and the compd. has very low soly. in water. We report the synthesis of an isomer (13) of NITP which has the desirable substitution pattern and is also sol. in very weak aq. base. The successful synthesis of 13 uses a nitrosation and cyclization of a substituted uracil (16), but earlier approaches from 5 and 12 yielded
 - the pyridoxanthine deriv. 6. The preparative use of nitro group displacement reactions from 8-nitrocaffeine is shown to be a useful entry to a range of 8-substituted caffeines and is utilized to obtain two derivs. of NITP which carry aliph. amine chains, i.e., 34 and 35.
- IT 152538-24-4
- (potential bioreductively activated hypoxia probes and radiosensitizers
- related to NITP)
- RN 152538-24-4 CAPLUS
- CN 1H-Purine-2,6-dione, 7+[4-[(3-amino-1,4-dioxido-1,2,4-benzotriazin-7-yl)oxy]butyl]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)
- *** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

L81 ANSWER 12 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1995:203474 CAPLUS

DN 122:81305

TI Preparation of ethers and esters of 2,3-bis(hydroxymethyl)quinoxaline 1,4-dioxide under phase-transfer catalysis conditions

AU Fridman, I. A.; Nikonova, I. V.; Koldobskii, G. I.

CS St. Peterburg. Gos. Tekhnol. Inst., Russia

SO Khim. Geterotsikl. Soedin. (1994), (6), 816-20 CODEN: KGSSAQ; ISSN: 0132-6244

DT Journal

LA Russian

AB The title compds. were prepd. by reaction of 2,3-bis(bromomethyl)quinoxaline 1,4-dioxide with phenols and carboxylic acids in phase-transfer systems. The catalytic activities of tetrabutylammonium

bromide and cetyltriethylammonium bromide were compared.

IT 160252-97-1P 160252-99-3P

RN 160252-97-1 CAPLUS

CN Benzaldehyde,

4,4'-[(1,4-dioxido-2,3-quinoxalinediyl)bis(methyleneoxy)]bis-(9CI) (CA INDEX NAME)

RN 160252-99-3 CAPLUS

CN Quinoxaline, 2,3-bis[(4-nitrophenoxy)methyl]-, 1,4-dioxide (9CI) (CA INDEX NAME)

L81 ANSWER 13 OF 40 CAPLUS COPYRIGHT 2000 ACS

ΑN 1994:681046 CAPLUS

DN 121:281046

ΤI Neutral ditopic receptors for adenosine monophosphate

Lacy, Stephen M.; Rudkevich, Dmitry M.; Verboom, Willem; Reinhoudt, David ΑU Ν.

CS Lab. Org. Chem., Univ. Twente, Enschede, 7500 AE, Neth.

SO Tetrahedron Lett. (1994), 35(32), 5953-6 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

Novel neutral ditopic receptors for AMP2- consisting of an immobilized AΒ Lewis acidic uranyl center covalently coupled to thymine are described.

ΙT 158793-00-1P 158793-01-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of neutral ditopic uranyl thymines as receptors for adenosine monophosphate)

RN 158793-00-1 CAPLUS

CN Benzaldehyde, 3-[4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)pyrimidinyl)butoxy]-2-(2-propenyloxy)- (9CI) (CA INDEX NAME)

Me
$$N - (CH_2)_4$$
 O $CH_2 - CH_2 - CH_2 - CH_2$

RN 158793-01-2 CAPLUS

Benzaldehyde, 3-[4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-CN pyrimidinyl)butoxy]-2-hydroxy- (9CI) (CA INDEX NAME)

Me
$$N - (CH_2)_4 - O - CHO$$

L81 ANSWER 14 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1994:164092 CAPLUS

DN 120:164092

TI Pyrimidinones as reversible metaphase arresting agents

AU Benneche, T.; Strande, P.; Oftebro, R.; Undheim, K.

CS Dep. Chem., Univ. Oslo, Oslo, N-0315, Norway

50 Eur. J. Med. Chem. (1993), 28(6), 463-72

CODEN: EJMCA5; ISSN: 0223-5234

DT Journal

LA English

GΙ

AB 5-Halo-N(1)-substituted 2(1H)-pyrimidinones, e.g. I (X = O, S, NCO2Et; n $\stackrel{-}{}$

0, 1; R = H, 2-Me, 4-Cl) were prepd. as agents to cause reversible arrest of mitosis during metaphase. In vitro data have been provided. It is suggested that reversible metaphase inhibitors can be used as synchronizing agents of cell-cycles by applying them in a sequential manner when a phase-specific cytotoxic drug is used in the treatment of diseases caused by uncontrolled rapidly proliferating cells. The active compds. are prepd. from 2-pyrimidinones by alkylation reactions. The key reactants are .alpha.-chloroalkyl ethers, sulfides and amides; methods

for

their syntheses have been described.

IT 100944-95-4P 100945-07-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as reversible metaphase arresting agent)

RN 100944-95-4 CAPLUS

CN Benzaldehyde, 4-[(5-chloro-2-oxo-1(2H)-pyrimidinyl)methoxy]- (9CI) (CA INDEX NAME)

Cl

RN 100945-07-1 CAPLUS

CN Benzaldehyde, 4-[[2-oxo-5-(trifluoromethyl)-1(2H)-pyrimidinyl]methoxy]-Searched by John Dantzma 703-308-4488 LA English

AB The i.p. LD50 values of the 14 quinazolones I (R = Cl, MeO, or NO2; R1 = H $^{\circ}$

or Br; R2 = H, Br, I; R3 = pyridyl or thiazolyl) tested in mice were .gtoreq.700 mg/kg. Almost all the compds. depressed the behavioral parameters measured. 2-(o-Methoxyphenoxymethyl)-3-(2'-thiazolyl)-4-quinazolone [73342-49-1] gave the best protection against pentylenetetrazol-induced seizures, decreasing the death rate by 60% when injected i.p. at 100 mg/kg 4 h before administration of the convulsant. Structure anticonvulsant activity relations are discussed.

IT 73342-54-8 73342-55-9

RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (pharmacol. of)

RN 73342-54-8 CAPLUS

CN 4(3H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 73342-55-9 CAPLUS

CN 4(3H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]-3-(2-thiazolyl)- (9CI) (CA INDEX NAME)

L81 ANSWER 30 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1976:164678 CAPLUS

DN 84:164678

TI Benzazoles. XXX. Amidomethylation of aromatic compounds with 1,3-bischloromethylbenzimidazolone and

1,3-bischloromethylbenzimidazolethi

one

AU Zinner, H.; Nitzsche, W.

CS Sekt. Chem., Univ. Rostock, Rostock, E. Ger.

SO J. Prakt. Chem. (1976), 318(1), 144-8 CODEN: JPCEAO

Journal

LA German

GΙ

DT

AB (Chloromethyl)benzimidazoles I (X = O, S; R = C1) (II) when treated with R1H (R1 = Ph, 4-MeC6H4, 2,5-Me2C6H3) in presence of AlC13 yielded 52--82%

I (R = R1). The reaction of II and phenoxides NaOR2 (R2 = Ph, 4-ClC6H4, C6Cl5) and KOC6H4NO2-4 gave 55-90% I (X = O, S; R = R2, OC6H4NO2-4).

IT 59103-49-0P

RN 59103-49-0 CAPLUS

CN 2H-Benzimidazole-2-thione, 1,3-dihydro-1,3-bis[(4-nitrophenoxy)methyl](9CI) (CA INDEX NAME)*

L81 ANSWER 31 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1976:38578 CAPLUS

DN 84:38578

Correlation analysis of Baker's studies on enzyme inhibition. 2. Chymotrypsin, trypsin, thymidine phosphorylase, uridine phosphorylase, thymidilate synthetase, cytosine nucleoside deaminase, dihydrofolate reductase, malate, glutamate, lactate, and glyceraldehyde-phosphate dehydrogenase

AU Yoshimoto, Masafumi; Hansch, Corwin

CS Dep. Chem., Pomona Coll., Claremont, Calif., USA

SO J. Med. Chem. (1976), 19(1), 71-98 CODEN: JMCMAR

DT Journal

LA English

The inhibitory activity of .apprx.1000 inhibitors of the title enzymes, .alpha.-chymotrypsin [9004-07-3], trypsin [9002-07-7], thymidine phosphorylase [9030-23-3], uridine phosphorylase [9030-22-2], thymidylate synthetase [9031-61-2], cytosine nucleoside deaminase [9025-06-3], dihydrofolate reductase [9002-03-3], malate dehydrogenase [9001-64-3], glutamate dehydrogenase [9001-46-1], glyceraldehyde-phosphate dehydrogenase [9001-50-7], and lactate dehydrogenase [9001-60-9], were formulated in 13 equations correlating chem. structure with inhibiting potency. Two types of regions in enzymes were defined by means of .pi. and molar refractive consts. The correlation equations showed that substituent effects are additive to a 1st approxn. Examples are given of use of the equations in comparing structural features of different systems.

IT 23572-67-0 26147-08-0 26147-09-1 26147-10-4 26159-11-5 57278-35-0

RL: BIOL (Biological study)

(cytosine nucleoside deaminase inhibition by, correlation anal. in relation to)

RN 23572-67-0 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-5-(3,4-dichlorophenyl)-1-[3-(2-nitrophenoxy)propyl]- (9CI) (CA INDEX NAME)

Searched by John Dantzma 703-308-4488

RN 26147-08-0 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[3-(2-nitrophenoxy)propyl]-5-phenyl- (9CI) (CA INDEX NAME)

RN 26147-09-1 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[3-(3-nitrophenoxy)propyl]-5-phenyl- (9CI) (CA INDEX NAME)

$$N = (CH_2)_3 = 0$$

RN 26147-10-4 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[3-(4-nitrophenoxy)propyl]-5-phenyl- (9CI) (CA INDEX NAME)

$$N = 0$$
 $N = 0$
 $N = 0$
 $N = 0$
 $N = 0$
 $N = 0$

RN 26159-11-5 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[3-(3-chloro-4-nitrophenoxy)propyl]-5-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

$$O_{2}N$$
 O_{1}
 $O_{2}N$
 $O_{2}N$
 O_{3}
 O_{1}
 O_{2}
 O_{2}
 O_{3}
 O_{2}
 O_{3}
 O_{3}
 O_{4}
 O_{5}
 O_{5}
 O_{7}
 O

RN 57278-35-0 CAPLUS

CN 2(1H)-Pyrimidinone, 4-Amino-1-[3-(2,4-dichloro-6-nitrophenoxy)propyl]-5-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

$$H_2N$$
 N
 O
 $C1$
 O_2N
 $C1$

L81 ANSWER 32 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1974:463633 CAPLUS

DN 81:63633

TI 5-Methyl-5-phenoxymethylhydantoins

IN Blaha, Ludvik; Weichet, Jaroslav

SO Czech., 4 pp. CODEN: CZXXA9

DT Patent

LA Czech

FAN.CNT 1

PATENT NO.	KIND	, DATE	APPLICATION NO.	DATE
CS 151744	В	19731119	CS 1971-357	19710119

GI For diagram(s), see printed CA Issue.

AB The title compds. I (R = OCH2Ph, OH, Me, OMe, Cl, NO2, NH2) were prepd.

in

PΙ

81-96% yield by reaction of RnC6H5-nOCH2COMe with (NH4)2CO3 and KCN in an aq.-alc. soln. 4 hr at room temp. and 15 hr at 45-50.degree. The aminophenoxy and hydroxyphenoxy derivs. were prepd., resp., by hydrogenation and debenzylation of the corresponding nitro and benzyloxy derivs. I had anticonvulsive and hypotensive activity.

IT 53012-39-8P 53012-40-1P 53012-44-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and anticonvulsant and antihypertensive activity of)

RN 53012-39-8 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-5-[(2-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

RN 53012-40-1 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

O
$$\frac{H}{N}$$
 $\frac{Me}{CH_2-O}$ $\frac{N}{NO_2}$

RN 53012-44-5 CAPLUS

CN 2,4-Imidazolidinedione, 5-[(4-amino-2-chlorophenoxy)methyl]-5-methyl-(9CI) (CA INDEX NAME)

IT 53012-43-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and redn. of)

RN 53012-43-4 CAPLUS

CN 2,4-Imidazolidinedione, 5-[(2-chloro-4-nitrophenoxy)methyl]-5-methyl-(9CI) (CA INDEX NAME)

L81 ANSWER 33 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1974:79600 CAPLUS

DN 80:79600

TI Model studies of the thymidylate synthetase reaction. Nucleophilic displacement of 5-p-nitrophenoxymethyluracils

Searched by John Dantzma 703-308-4488

AU Pogolotti, Alfonso L., Jr.; Santi, Daniel V.

CS Dep. Biochem. Biophys., Univ. California, San Francisco, Calif., USA

SO Biochemistry (1974), 13(3), 456-66

CODEN: BICHAW

DT Journal

LA English

Nucleophilic displacement reactions of 5-p-nitrophenoxymethyluracil and ABits N-alkylated derivs. were examd. to provide insight into the mechanism by which thymidylate synthetase catalyzes hydride transfer from 5,10-methylenetetrahydrofolate to the Me group of thymidylate. All reactions appear to proceed by formation of highly reactive intermediates having an exocyclic methylene group at the 5-position of the heterocycle rather than direct displacement (SN2) of the leaving group. The driving force for the expulsion of the leaving group and formation of such intermediates may be provided by the N-1 anion, where possible, or by attack of a nucleophile at the 6-position of the heterocycle when the 1-position is alkylated. Direct support for the proposed mechanisms was obtained by evaluation of secondary 2H isotope effects of reactants possessing 2H at the 5-methylene C or the 6-position of the heterocycle. The mechanism involving nucleophilic attack at the 6-position of the heterocycle is analogous to that obsd. in model studies of other reactions

catalyzed by this enzyme, and permits a unified mechanism for catalysis, which is supported by all chem. and biochem. data at hand, to be proposed.

Discussion is presented which argues against the existence of a thymidylyl-tetrahydrofolate intermediate in the reaction pathway leading to products.

IT 32078-95-8 32078-98-1 32079-01-9 32079-07-5 52458-45-4

RL: RCT (Reactant)

(hydrolysis of, thymidylate synthetase reaction mechanism in relation to)

RN 32078-95-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$O \longrightarrow H$$
 $N \longrightarrow CH_2 - O$
 $O \longrightarrow N$
 $O \longrightarrow N$

RN 32078-98-1 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 1-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

32079-01-9 CAPLUS 2,4(1H,3H)-Pyrimidinedione, 3-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) CN (CA INDEX NAME)

$$\begin{array}{c|c} O_{\text{obs}} & H \\ \hline N \\ N \\ \hline N \\ O \\ \end{array}$$

32079-07-5 CAPLUS RN 2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-5-[(4-nitrophenoxy)methyl]-CN (9CI) (CA INDEX NAME)

Me
$$N = CH_2 = O$$

52458-45-4 CAPLUS RN 2,4(1H,3H)-Pyrimidinedione, 1-(3-aminopropyl)-3-methyl-5-[(4-CN nitrophenoxy)methyl]-, acetate (9CI) (CA INDEX NAME)

СМ 1

CRN 52458-44-3 CMF C15 H18 N4 O5

CM 2

CRN 64-19-7 CMF C2 H4 O2

IT 52458-50-1P

RN 52458-50-1 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione,

1-[3-[[(4-methoxyphenyl)diphenylmethyl]amino]p ropyl]-3-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{O} \\ & \text{N} \end{array} \begin{array}{c} \text{O} \\ & \text{N} \end{array} \begin{array}{c} \text{Ph} \\ & \text{OMe} \end{array}$$

L81 ANSWER 34 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1972:419649 CAPLUS

DN 77:19649

TI 1-Aryl-5-(hydroxyalkyl)hydantoins as central nervous system-affecting agents

IN Skorcz, Joseph A.; Suh, John T.

PA Colgate-Palmolive Co.

SO U.S., 4 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

703-308-4488

Searched by John Dantzma

19720321 US 1968-778750 19681125 Α PΤ US 3651079

For diagram(s), see printed CA Issue. GΙ

The arylhydantoins I (R = NO2, NH2; R1 = H, Ac; R2 = H, Me), useful as AΒ central nervous system depressants and as antihypertensives, wereprepd.

by cyclizing II with KCN-(NH4)2CO3. Thus, 22.5 g of II was refluxed with 9.8

q KCN and 57.7 g (NH4)2CO3 in 50% aq. EtOH to give I (R = NO2, R1 = R2 = H); the related 5-(2-methoxy-4-nitrophenoxy)methyl-5-methylhydantoin is also formed but may be rearranged by further treatment with (NH4)2-CO3-KCN

to I. I have i.p. LD50 in mice <500 mg/kg.

ΙT 29482-31-3P

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

29482-31-3 CAPLUS RN

2,4-Imidazolidinedione, 5-[(2-methoxy-4-nitrophenoxy)methyl]-5-methyl-CN (9CI) (CA INDEX NAME)

L81 ANSWER 35 OF 40 CAPLUS COPYRIGHT 2000 ACS

1971:405838 CAPLUS AN

75:5838 DN

Nucleophilic substitution reactions of 5-acetoxymethyl and TΙ 5-p-nitrophenoxymethyluracils

ΑU

Santi, Daniel V.; Pogolotti, A. L., Jr. Dep. Chem., Univ. California, Santa Barbara, Calif., USA

J. Heterocycl. Chem. (1971), 8(2), 265-72 SO CODEN: JHTCAD

DTJournal

LAEnglish

The synthesis of 5-(acetoxymethyl)- and 5-(p-nitrophenoxymethyl)uracils AΒ and their nucleophilic substitution reactions with MeONa and NaBH4 are reported. These reactions all appear to involve intermediates with carbonium ion character, the formation of which are dependent upon structural features of the heterocycle. Most facile reactions occur when the 1-position of the heterocycle can accommodate a neg. charge to assist in the formation of highly reactive 5-methyleneuracil intermediates. Where ionization is precluded, as with 1-methyl derivs. displacements are retarded but may be assisted by addn. of a nucleophile to the 6-position of the heterocycle. Analogous 1,3-dialkylpyrimidines may react with nucleophiles at the 4-carbonyl group to give anomalous products. Biol. connotations of these reactions are discussed.

32078-95-8P 32078-98-1P 32079-01-9P IT32079-07-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

32078-95-8 CAPLUS RN

Searched by John Dantzma 703-308-4488

CN 2,4(1H,3H)-Pyrimidinedione, 5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$O = H$$
 HN
 $CH_2 = O$
 NO_2

32078-98-1 CAPLUS RN

2,4(1H,3H)-Pyrimidinedione, 1-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & \\ \hline \\ N & \\ \hline \\ N & \\ CH_2-O \end{array}$$

32079-01-9 CAPLUS RN

2,4(1H,3H)-Pyrimidinedione, 3-methyl-5-[(4-nitrophenoxy)methyl]- (9CI) CN (CA INDEX NAME)

32079-07-5 CAPLUS RN

2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl-5-[(4-nitrophenoxy)methyl]-CN (9CI)

(CA INDEX NAME)

Searched by John Dantzma 703-308-4488

```
L81 ANSWER 36 OF 40 CAPLUS COPYRIGHT 2000 ACS
    1970:531306 CAPLUS
ΑN
DN
    73:131306
ΤI
    Alkylaryloxy alanines, central nervous system stimulants
    Suh, John T.; Skorcz, Joseph A.
ΙN
PA
    Colgate-Palmolive Co.
SO
    U.S., 4 pp.
    CODEN: USXXAM
DT
    Patent
LA
    English
FAN.CNT 1
    LIS 3529019 APPLICATION NO. DATE
                                        _____
    US 3529019 A 19700915 US 1968-723605 19680423
PΙ
    The title compds. are prepd. by reacting a substituted ketone with
AB
     (NH4)2CO3 and KCN in 50 aq. EtOH to form a 5-alkyl-5-(2-
    alkoxyphenoxy) methylhydantoin which with Ba(OH)2.8H2O forms
    2-alkyl-3-(2-alkoxyphenoxy)alanine. Thus, .omicron.-
    methoxyphenoxyacetone, (NH4)2CO3, and KCN in 50% aq. EtOH refluxed 24 hr
    and acidified to pH 2 yields 5-methyl-5-(2-methoxyphenoxy)methylhydantion
     (I), m. 138.5-40.degree. (aq. EtOH). I and Ba(OH)2.8H2O in H2O refluxed
    70 hr and acidified forms 2-methyl-3-(2-methoxyphenoxy)alanine, m.
    250-2.degree. (aq. Me2CO); Me ester.HCl, m. 120-4.degree., Et ester b0.1
    115.degree.. Also prepd. are 10 similar compds.
    29482-31-3P 29482-32-4P
IT
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of)
    29482-31-3 CAPLUS
RN
    2,4-Imidazolidinedione, 5-[(2-methoxy-4-nitrophenoxy)methyl]-5-methyl-
CN
    (9CI) (CA INDEX NAME)
```

RN 29482-32-4 CAPLUS

CN Hydantoin, 5-[(4-amino-2-methoxyphenoxy)methyl]-5-methyl-, monohydrochloride (8CI) (CA INDEX NAME)

● HCl

L81 ANSWER 37 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1970:3708 CAPLUS

DN 72:3708

TI Irreversible enzyme inhibitors. CLXII. Hydrophobic bonding to cytosine nucleoside deaminase with 1-substituted 5-arylcytosines

AU Baker, Bernard Randall; Kelley, James L.

CS Univ. of California, Santa Barbara, Calif., USA

SO J. Med. Chem. (1969), 12(5), 1039-45 CODEN: JMCMAR

DT Journal

LA English

1-Phenoxypropyl-5-phenylcytosine (I) was previously reported to be an AΒ inhibitor of cytosine nucleoside deaminase that was complexed one-fourth as well as the substrate, 2'-deoxycytidine. In order to enhance the activity of I, 41 variants were synthesized for e valuation: (a) the 1-phenoxypropyl moiety was as good or better than fiv e other 1-substituents studied; (b) when the 5-phenyl group was substituted with ten different groups, optimum binding occurred with the 3,4-Cl2 substituents; (c) 15 different substituents on the phenoxy moiety gave little change in binding, but showed good bulk tolerance for the large benzamido substituent; (d) five combinations of the substituents on the 2,4-positions of the pyrimidine moiety gave optimum binding with the 2-oxo-4-thione combination. Among the best inhibitors derived from 5-(3,4-dichlorophenyl)cytosine were the 1-(p-chlorophenoxypropyl) and 1-(m-benzamidophenoxypropyl) derivs. which were complexed three-fold better to the enzyme than the substrate.

IT 23572-67-0P 26147-08-0P 26147-09-1P

26147-10-4P 26159-09-1P 26159-11-5P

26159-12-6P 26159-17-1P 26159-18-2P

26159-19-3P 26250-41-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of)

RN 23572-67-0 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-5-(3,4-dichlorophenyl)-1-[3-(2-nitrophenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 26147-08-0 CAPLUS 2(1H)-Pyrimidinone, 4-amino-1-[3-(2-nitrophenoxy)propyl]-5-phenyl- (9CI) CN (CA INDEX NAME)

$$N = 0$$
 $N = 0$
 $N =$

RN 26147-09-1 CAPLUS 2(1H)-Pyrimidinone, 4-amino-1-[3-(3-nitrophenoxy)propyl]-5-phenyl- (9CI) CN (CA INDEX NAME)

26147-10-4 CAPLUS RN 2(1H)-Pyrimidinone, 4-amino-1-[3-(4-nitrophenoxy)propyl]-5-phenyl- (9CI) CN (CA INDEX NAME)

26159-09-1 CAPLUS RN Cytosine, 5-(3,4-dichlorophenyl)-1-[3-(p-nitrophenoxy)propyl]- (8CI) (CA CN INDEX NAME)

RN 26159-11-5 CAPLUS

CN 2(1H)-Pyrimidinone, 4-amino-1-[3-(3-chloro-4-nitrophenoxy)propyl]-5-(3,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

$$O_2N$$
 O_1
 O_2N
 O_3
 O_4
 O_5
 O_5
 O_7
 $O_$

RN 26159-12-6 CAPLUS

CN Cytosine,

1-[3-(4,5-dichloro-2-nitrophenoxy)propyl]-5-(3,4-dichlorophenyl)(8CI) (CA INDEX NAME)

$$H_2N$$
 N
 O
 $C1$
 O_2N
 $C1$

RN 26159-17-1 CAPLUS

CN Cytosine, 1-[3-(o-aminophenoxy)propyl]-5-(3,4-dichlorophenyl)- (8CI) (CA INDEX NAME)

Searched by John Dantzma

703-308-4488

RN 26159-18-2 CAPLUS

CN Cytosine, 1-[3-(m-aminophenoxy)propyl]-5-(3,4-dichlorophenyl)- (8CI) (CF INDEX NAME)

RN 26159-19-3 CAPLUS

CN Cytosine, 1-[3-(p-aminophenoxy)propyl]-5-(3,4-dichlorophenyl)- (8CI) (CA INDEX NAME)

$$O - (CH_2)_3 - N$$
 $O - (CH_2)_3 - N$
 $O - (CH_2)_$

RN 26250-41-9 CAPLUS

CN Cytosine, 5-(3,4-dichlorophenyl)-1-[3-(m-nitrophenoxy)propyl]- (8CI) (CA INDEX NAME)

L81 ANSWER 38 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1969:68293 CAPLUS

DN 70:68293

Irreversible enzyme inhibitors. CXLIII. Active-site-directed irreversible inhibitors of dihydrofolic reductase derived from 5-[3-(p-aminophenoxy)propyl]-2,4-diamino-6-methylpyrimidine with a terminal sulfonyl fluoride

AU Baker, Bernard Randall; Meyer, Rich B., Jr.

CS Univ. of California, Santa Barbara, Calif., USA

SO J. Med. Chem. (1969), 12(1), 108-11

CODEN: JMCMAR

DT Journal

LA English

AB 2,4-Diamino-5-[3-[p-(m-fluorosulfonylbenzamido)phenoxy]propyl]-6methylpyrimidine (I) and 3 variants in the benzamido moiety have been
synthesized via the intermediate 2-amino-6-methyl-5-[3-(pnitrophenoxy)propyl]-4-pyrimidinol and 5-[3-(p-aminophenoxy)propyl]-2,4diamino-6-methylpyrimidine; the key reaction was azide displacement of
the

Cl of 2-acetamido-4-chloro-6-methyl-5-[3

- (p-nitrophenoxy) propyl] pyrimidin

e followed by redn. of the azidopyrimidine to the 4-aminopyrimidine,

the usual NH3 displacement caused cleavage of the nitrophenoxy side chain.

I met all the criteria for in vivo evaluation as an irreversible inhibitor

of dihydrofolic reductase, but was inactive in vivo because of poor cell-wall penetration. N-[p-(4,6-Diamino-2,2-dimethyl-1,2-dihydro-s-triazin - 1 -yl)hydrocinnamoyl]sulfanilyl fluoride showed good

of the cell wall and good in vivo activity, but was not a selective irreversible inhibitor of dihydrofolic reductase since it also inactivated

the enzyme from mouse liver, spleen, and intestine.

IT 21428-08-0P

RN 21428-08-0 CAPLUS

CN Acetamide, N-[4-hydroxy-6-methyl-5-[3-(p-nitrophenoxy)propyl]-2-pyrimidinyl]- (8CI) (CA INDEX NAME)

L81 ANSWER 39 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1967:112442 CAPLUS

DN 66:112442

TI Irreversible enzyme inhibitors. LXIX. Candidate active-site-directed irreversible inhibitors of dihydrofolic reductase. Bromoacyl derivatives of 5-(p-aminophenoxypropyl-2,4,6-triaminopyrimidines

AU Baker, Bernard Randall; Santi, Daniel V.

CS Univ. of California, Santa Barbara, Calif., USA

SO J. Pharm. Sci. (1967), 56(3), 380-4 CODEN: JPMSAE

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB cf. CA 66, 26263a, 62158d. 5-(p-Amino-phenoxypropyl)-2,4,6triaminopyrimidine (I) was synthesized by alkylation of malononitrile by 3-bromopropyl p-nitrophenyl ether, followed by ring closure with guanidine Searched by John Dantzma 703-308-4488 and catalytic redn. of the nitro group. Selective haloacylation of the aromatic amino group of I was accomplished by protonation of the triaminopyrimidine moiety of I with acetic acid. Treatment with the anhydrides of bromoacetic acid, p-bromoacetamido-phenylbutyric acid, and N-bromoacetyl-.beta.-alanine gave the pure bromoacyl derivs. These three compds. were good reversible inhibitors of dihydrofolic reductase, but failed to show irreversible inhibition; these failures are attributed to the phenoxypropyl group of the inhibitors being complexed with a hydrophobic region on the enzyme, a region not apt to have groups that could form a covalent bond. 27 references.

IT 15761-66-7P

RN 15761-66-7 CAPLUS

CN 4-Pyrimidinol, 2-amino-6-methyl-5-[3-(p-nitrophenoxy)propyl]- (8CI) (CA INDEX NAME)

$$H_2N$$
 N O NO_2 Me

L81 ANSWER 40 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1967:26263 CAPLUS

DN 66:26263

TI Irreversible enzyme inhibitors. LXVIII. 2-Amino-5-(p-bromoacetamidophenoxypropyl)-6-phenyl-4-pyrimidinol, an active-site-directed irreversible inhibitor of dihydrofolic reductase

AU Baker, Bernard Randall; Shapiro, Howard S.

CS Univ. of California, Santa Barbara, Calif., USA

SO J. Pharm. Sci. (1966), 55(12), 1422-5 CODEN: JPMSAE

DT Journal

LA English

AB cf. preceding abstr.

2-Amino-5-(p-bromoacetamidophenoxypropyl)-6-phenyl-4-

pyrimidinol (I), when incubated with dihydrofolic reductase at

37.degree.,

inactivated the enzyme with a halflife of about $45~\mathrm{min}$. In contrast, iodoacetamide and p-bromoacetamidophenylbutyric acid at the same conc. no inactivation of the enzyme in the same time. An interesting contrast to

was the 6-Me analog of I which inactivated the enzyme at about one-seventh

the rate of I. This result gives unequivocal support for a previous suggestion that 6-methylpyrimidines and 6-phenylpyrimidines do not reversibly complex with dihydrofolic reductase in the same manner, else I and its 6-Me analog should have inactivated the enzyme at the same rate

at

Τ

equal concns. of reversible complex. These expts. are best explained on the basis of active-site-directed irreversible inhibition of dihydrofolic reductase.

14937-56-5P 14937-58-7P 15065-48-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 14937-56-5 CAPLUS

4-Pyrimidinol, 2-amino-5-[3-(p-nitrophenoxy)propyl]-6-phenyl- (8CI) (CA CN INDEX NAME)

 H_2N

14937-58-7 CAPLUS RN

4-Pyrimidinol, 2-amino-5-[3-(p-aminophenoxy)propyl]-6-phenyl-, dihydrochloride (8CI) (CA INDEX NAME)

Ph

● 2 HCl

RN 15065-48-2 CAPLUS

4-Pyrimidinol, 2-amino-5-[3-(p-aminophenoxy)propyl]-6-methyl-, CN dihydrochloride (8CI) (CA INDEX NAME)

 H_2N

2 HCl

\Rightarrow d 1-6 all hitstr

L82 ANSWER 1 OF 6 CAOLD COPYRIGHT 2000 ACS

AN CA63:16463e CAOLD

TI protective groups in peptide chemistry

AU Wieland, Theodor

IT 3970-00-1 3970-05-6 3970-06-7 3970-07-8 3970-08-9 3979-44-0 4598-50-9 6344-12-3 **100197-24-8**

IT 100197-24-8

RN 100197-24-8 CAOLD

CN Salicylaldehyde, 5-chloro-, 0,0'-[(3,6-dioxo-2,5-piperazinediyl)dimethylene]dioxime (7CI) (CA INDEX NAME)

L82 ANSWER 2 OF 6 CAOLD COPYRIGHT 2000 ACS

AN CA61:16058c CAOLD

TI mechanism of cycloserine dimerization in the presence of 5-chlorosalicylaldehyde

AU Stammer, Charles H.; McKinney, J. D.

IT 635-93-8 2658-23-3 92440-95-4 93898-35-2 **100197-24-8**

IT 100197-24-8

RN 100197-24-8 CAOLD

CN Salicylaldehyde, 5-chloro-, 0,0'-[(3,6-dioxo-2,5-piperazinediyl)dimethylene]dioxime (7CI) (CA INDEX NAME)

L82 ANSWER 3 OF 6 CAOLD COPYRIGHT 2000 ACS

AN CA61:14672d CAOLD

TI Schiff base of cycloserine

AU Stammer, Charles H.

IT 6344-12-3 91768-75-1 92575-39-8 **100197-24-8**

IT 100197-24-8

RN 100197-24-8 CAOLD

CN Salicylaldehyde, 5-chloro-, 0,0'-[(3,6-dioxo-2,5piperazinediyl)dimethylene]dioxime (7CI) (CA INDEX NAME)

L82 ANSWER 4 OF 6 CAOLD COPYRIGHT 2000 ACS

CA59:7516a CAOLD

ΤI bis(2-chloroethyl)amines, derivs. of urea and thiourea

ΑU

Berlin, A. Ya.; Levi, I. S. 6720-60-1 88784-24-1 91562-06-0 91646-33-2 91646-34-3 91721-27-6 IT92021-73-3 93137-10-1 93137-11-2 93868-93-0 93994-77-5 94025-18-0 94025-19-1 94691-27-7 95125-78-3 97118-40-6 97118-41-7 96434-00-3 97491-77-5 97598-06-6 97791-07-6 98472-85-6

ΙT 98472-85-6

98472-85-6 CAOLD RN

2-Imidazolidinethione, 1-benzoyl-3-[2-(picryloxy)ethyl]- (7CI) (CA INDEX CN NAME)

L82 ANSWER 5 OF 6 CAOLD COPYRIGHT 2000 ACS

ΑN CA54:16655b CAOLD

schistosomicidal and toxic effects of some N-p-aminophenoxyalkylamides ΤI

Collins, Raymond F.; Davis, M.; Edge, N. D.; Hill, J.; Reading, H. W.; Searched by John Dantzma 703-308-4488

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Turnbull, E. R.
IT 100317-01-9 100800-28-0 100840-50-4 100861-96-9 100862-15-5 100958-17-6
     101116-78-3 101264-04-4 101275-49-4 101351-09-1 101354-76-1 101438-70-4
     102008-47-9 102008-49-1 102008-50-4 102008-63-9 102008-71-9 102016-51-3
     102081-66-3 102163-66-6 102164-43-2 102164-84-1 102165-68-4 102167-11-3
     102178-85-8 102181-76-0 102181-79-3 102181-80-6 102319-97-1 102375-33-7
     102375-34-8 102453-56-5 102457-61-4 102457-85-2 102552-65-8 102556-31-0
     102667 - 13 - 0 \ 102759 - 82 - 0 \ 102809 - 98 - 3 \ 102812 - 68 - 0 \ 102886 - 68 - 0 \ 102955 - 75 - 9
     103050-73-3 103161-39-3 103168-96-3 103277-13-0 103387-97-9 103388-57-4
     103388-58-5 103388-59-6 103503-82-8 103507-77-3 103508-20-9 103509-47-3
     103640-92-2 103643-77-2 103643-81-8 103644-25-3 103649-48-5 103758-22-1
     104295-14-9 106165-47-3 106653-05-8 107627-36-1 107778-44-9 107918-76-3 108367-29-9 108368-14-5 108477-52-7 108984-25-4 109806-61-3
     109806-62-4 109808-49-3 111440-64-3 111498-38-5 112971-97-8 113752-63-9
     113861-35-1 114889-00-8 115294-19-4 118634-18-7 119299-66-0 119299-67-1
     123104-28-9 124105-90-4 132493-51-7
ΙT
     106653-05-8
RN
     106653-05-8 CAOLD
CN
     Barbituric acid, 1-[5-(p-aminophenoxy)pentyl]- (6CI) (CA INDEX NAME)
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L82 ANSWER 6 OF 6 CAOLD COPYRIGHT 2000 ACS
     CA54:7613f CAOLD
TΙ
     chemotheraphy of schistosomiasis - (III) N-(p-aminophenoxyalkyl)amides,
     -imides, and -sulfonamides
ΑU
     Ashley, Julius N.; Collins, R. F.; Davis, M.; Sirett, N. E.
     904-10-9 25934-63-8 98395-61-0 99982-26-0 100055-08-1 100254-69-1
     100317 - 01 - 9 \ 100528 - 33 - 4 \ 100531 - 60 - 0 \cdot 100720 - 45 - 4 \ 100723 - 12 - 4 \ 100840 - 50 - 4 
     100861-96-9 100958-17-6 100973-99-7 101116-78-3 101264-04-4
     101269-11-8 101270-40-0 101275-49-4 101275-78-9 101275-79-0 101289-48-9
     101351-09-1 101354-76-1 101438-70-4 101497-19-2 101575-26-2
     101579-81-1 101585-23-3 101586-61-2 101587-15-9 101587-77-3
     101715-77-9 101715-90-6 101728-11-4 101732-28-9 101738-01-6 101738-05-0
     101738-09-4 101740-15-2 101783-33-9 101785-64-2 101786-01-0 101786-05-4
     101793-62-8 101793-97-9 101868-63-7 101878-40-4 101936-15-6 101939-29-1
     101939-56-4 102003-31-6 102008-48-0 102008-50-4 102008-63-9 102009-08-5
    102016-51-3 102017-05-0 102017-11-8 102081-56-1 102081-66-3 102160-77-0
    102163-65-5 102164-43-2 102164-84-1 102164-85-2 102165-68-4 102165-87-7
    102167-62-4 102172-69-0 102178-85-8 102182-06-9 102182-10-5 102182-12-7
    102240-34-6 102316-95-0 102317-32-8 102318-51-4 102320-11-6 102375-33-7
    102443-46-9 102457-85-2 102470-72-4 102556-31-0 102600-32-8 102659-73-4
    102660-64-0\ 102667-13-0\ 102810-16-2\ 102812-68-0\ 102952-06-7\ 102954-32-5
    103046-20-4 103047-05-8 103050-73-3 103100-48-7 103168-96-3 103210-03-3
    103211-66-1 103267-38-5 103388-57-4 103388-58-5 103390-68-7 103395-65-9
    103403-08-3 103503-82-8 103506-35-0 103506-54-3 103507-12-6 103508-20-9
                   Searched by John Dantzma 703-308-4488
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103640-67-1 103641-74-3 103642-45-1 103644-05-9 103644-87-7 103694-53-7 103758-22-1 103990-75-6 104176-82-1 104295-14-9 105838-73-1 106165-47-3 106273-32-9 106381-78-6 106653-05-8 107056-83-7 107419-24-9 107627-36-1 107778-44-9 107918-76-3 108240-51-3 108240-60-4 108246-09-9 108367-29-9 108368-14-5 108368-15-6 108851-37-2 108884-20-4 109037-66-3 109094-52-2 109158-47-6 109399-23-7 109446-11-9 109477-40-9 109557-29-1 109566-95-2 109813-10-7 109814-74-6 109847-65-6 109935-41-3 110530-70-6 110534-68-4 110938-45-9 111142-06-4 111241-28-2 111440-64-3 111978-34-8 112071-51-9 112271-84-8 112624-89-2 112625-46-4 112746-43-7 112971-97-8 113039-22-8 113184-12-6 113325-63-6 113752-63-9 113861-35-1 114034-13-8 114277-18-8 115294-19-4 116604-72-9 116999-72-5 117123-84-9 119417-09-3 119597-35-2 120547-80-0 121622-54-6 122337-11-5 124105-90-4 131240-28-3 131977-44-1 132568-41-3 100973-99-7 101579-81-1 106653-05-8 100973-99-7 CAOLD

TT

RN

Barbituric acid, 1-[5-(p-nitrophenoxy)pentyl]- (6CI) (CA INDEX NAME) CN

RN 101579-81-1 CAOLD

Barbituric acid, 5-acetyl-1-[5-(p-nitrophenoxy)pentyl]- (6CI) (CA INDEX CN NAME)

RN 106653-05-8 CAOLD

CN Barbituric acid, 1-[5-(p-aminophenoxy)pentyl]- (6CI) (CA INDEX NAME)

```
L45
               0 S L35 SSS SAM SUB=L41
 L46
                 SCR 1839 AND 1993 AND 2004 AND 103
 L47
               1 S L26 AND L46 SSS SAM SUB=L41
 L48
          529658 S L41 AND NCNC2/ESS
 L49
               1 S L26 AND L46 SSS SAM SUB=L48
 L50
          298725 S NCNC2/ES AND O/ELS AND NRS>1
 L51
               1 S L26 SSS SAM SUB=L50
 L52
          285783 S NC2NC2/ESS AND O/ELS AND NRS>1
 L53
          284158 S L52 NOT SEQ/FA
 L54
               0 S L25 SSS SAM SUB=L53
 L55
          598235 S NCNC2/ESS AND O/ELS AND NRS>1
 L56
          529658 S L55 NOT SEQ/FA
 L57
               1 S L26 AND L46 SSS SAM SUB=L56
          585983 S NCNC3/ESS AND O/ELS AND NRS>1
L58
L59
          576308 S L58 NOT SEQ/FA
L60
               0 S L35 SSS SAM SUB=L59
               0 S L35 AND L46 SSS SAM SUB=L59
L61
L62
                 SCR 1839 AND 1993 AND 2004 AND 150
L63
               2 S L26 AND L62 SSS SAM SUB=L56
L64
                 SCR 1950
L65
              1 S L35 OR L26 AND L62 SSS SAM SUB=L41
L66
                SCR 1950
L67
              1 S L26 AND L62 AND L66 SSS SAM SUB=L56
L68
              3 S L26 AND L62 NOT L66 SSS SAM SUB=L56
L69
              0 S L35 AND L46 SSS SAM SUB=L59
L70
              0 S L35 AND L46 AND L66 SSS SAM SUB=L59
L71
              0 S L35 AND L46 NOT L66 SSS SAM SUB=L59
L72
            110 S L35 AND L46 NOT L66 SSS FUL SUB=L59
L73
             21 S L35 AND L46 AND L66 SSS FUL SUB=L59
L74
             82 S L26 AND L62 AND L66 SSS FUL SUB=L56
L75
            220 S L26 AND L62 NOT L66 SSS FUL SUB=L56
L76
            481 S L25 SSS FUL SUB=L53
                SAV QAZ535A/A L72
                SAV QAZ535B/A L73
                SAV QAZ535C/A L74
                SAV QAZ535D/A L75
                SAV QAZ535E/A L76
L77
            914 S L72-L76
L78
                STR L25
L79
              3 S L78 SSS SAM SUB=L77
L80
            135 S L78 SSS FUL SUB=L77
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L81
             40 S L80
     FILE 'CAOLD' ENTERED AT 14:58:00 ON 05 JUL 2000
L82
              6 S L80
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=> d his

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(FILE 'HOME' ENTERED AT 13:31:57 ON 05 JUL 2000)
      FILE 'HCAPLUS' ENTERED AT 13:32:02 ON 05 JUL 2000
 L1
              23 S LOHRAY V?/AU
 L2
              84 S LOHRAY B?/AU
 L3
               7 S PARASELLI R?/AU
 L4
               4 S GURRAM R?/AU
 L5
              40 S RAMANUJAM R?/AU
             160 S CHAKRABARTI R?/AU
 L7
               6 S PAKALA S?/AU
 L8
               2 S L1 AND L2 AND L3 AND L4 AND L5 AND L6 AND L7
                 SELECT RN L8 1-2
      FILE 'REGISTRY' ENTERED AT 13:33:17 ON 05 JUL 2000
 L9
             116 S E1-116
      FILE 'HCAPLUS' ENTERED AT 13:33:55 ON 05 JUL 2000
 L10
               2 S L8 AND L9
      FILE 'REGISTRY' ENTERED AT 13:36:42 ON 05 JUL 2000
L11
L12
               6 S L11
L13
                STR L11
L14
               6 S L13
L15
                STR L13
L16
               0 S L15 AND L13
L17
                SCR 1839 AND 2004 AND 1993
L18
              0 S L15 AND L13 AND L17
L19
             6 S L13 AND L17
L20
                SCR 150 AND 1839 AND 2004 AND 1993
L21
             10 S L13 AND L20
L22
                STR L13
L23
              3 S L22 AND L20
L24
              0 S L22 AND L15 AND L20
L25
                STR L22
L26
                STR L25
L27
              0 S L25 OR L26 AND L20
L28
               SCR 1951
L29
              2 S L25 OR L26 AND L20 AND L28
L30
              1 S L25 OR L26 AND L20 NOT L28
L31
                SCR 1950
L32
              1 S L25 OR L26 AND L20 NOT L31
L33
              0 S L25 OR L26 AND L20 AND L31
L34
                SCR 146 OR 150
L35
                STR L25
L36
              0 S (L25 OR L26 OR L35) AND L34 AND L17
        1269154 S (NC2NC2 OR NCNC3 OR NCNC2)/ESS AND O/ELS AND NRS>1
L37
              1 S (L25 OR L26 OR L35) AND L34 AND L17 SSS SAM SUB=L37
L38
L39
                STR
              0 S L39 AND (L25 OR L26 OR L35) AND L34 AND L17 SSS SAM SUB=L37
L40
L41
        1197292 S L37 NOT SEQ/FA
              0 S L39 AND (L25 OR L26 OR L35) AND L34 AND L17 SSS SAM SUB=L41
L42
L43
              0 S L25 SSS SAM SUB=L41
L44
              2 S L26 SSS SAM SUB=L41
                   Searched by John Dantzma
                                              703-308-4488
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QAZI 09/535387

Page 3

=> d que 180

L25

STR

CH2G2--O--Cy--G3 @6 7 8 9 10

CH=N--OH @11 12 13

25 26 OH O CH2 CH - C --- 0--- G4 @19 20 21 22 27

Ak @28

23 24 33 34 OH O Χ 0 CH2-N--C-NH2 CH2-CH-C---O----G4 @14 15 16 17 @29 30 31 32 35

@37 36 C N C @38 40

CH2-NH-OH 042 43 44

REP G2 = (0-7) CH2 VAR G3=CHO/NO2/NH2/11/14/19/29/42 VAR G4=H/28VPA 6-37/38 U NODE ATTRIBUTES: CONNECT IS E1 RC AT 28 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE

CH2G2-O-Cy-G3 CH=N-OH @6 7 8 9 10 @11 12 13

25 26 OH O CH2 CH- C-- 0-- G4 @19 20 21 22 27

Ak 028

23 24 ОН О CH2 N==C==NH2 014 15 16 17

33 34 х о

037 @36 C N C @38 $C \sim \sim N$ 41

CH2-NH -OH 042 43 44

REP G2 = (0-7) CH2 VAR G3=CHO/NO2/NH2/11/14/19/29/42 VAR G4=H/28 VPA 6-37/38/36 U NODE ATTRIBUTES: CONNECT IS E1 RC AT 28 DEFAULT MLEVEL IS ATOM

QAZI

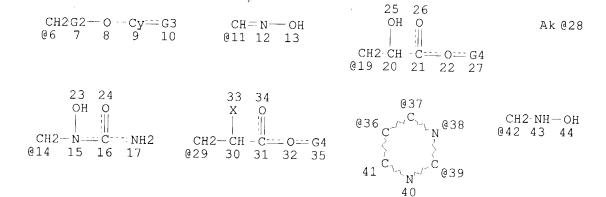
09/535387

Page 4

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 37

STEREO ATTRIBUTES: NONE L35 STR



REP G2 = (0-7) CH2 VAR G3=CHO/NO2/NH2/11/14/19/29/42 VAR G4=H/28VPA 6-39/38/37/36 U NODE ATTRIBUTES: CONNECT IS E1 RC AT 28 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 38

STEREO ATTRIBUTES: NONE L46 SCR 1839 AND 1993 AND 2004 AND 103 L52 285783 SEA FILE=REGISTRY ABB=ON PLU=ON NC2NC2/ESS AND O/ELS AND NRS>1 L53 284158 SEA FILE=REGISTRY ABB=ON PLU=ON L52 NOT SEQ/FA 598235 SEA FILE=REGISTRY ABB=ON PLU=ON NCNC2/ESS AND O/ELS AND L55 NRS>1 529658 SEA FILE=REGISTRY ABB=ON PLU=ON L55 NOT SEQ/FA L56 585983 SEA FILE=REGISTRY ABB=ON PLU=ON NCNC3/ESS AND O/ELS AND L58 NRS>1 576308 SEA FILE=REGISTRY ABB=ON PLU=ON L58 NOT SEQ/FA L59 L62 SCR 1839 AND 1993 AND 2004 AND 150 L66 SCR 1950 L72 110 SEA FILE=REGISTRY SUB=L59 SSS FUL L35 AND L46 NOT L66 L73 21 SEA FILE=REGISTRY SUB=L59 SSS FUL L35 AND L46 AND L66 L74 82 SEA FILE=REGISTRY SUB=L56 SSS FUL L26 AND L62 AND L66 220 SEA FILE=REGISTRY SUB=L56 SSS FUL L26 AND L62 NOT L66 L75 L76 481 SEA FILE=REGISTRY SUB=L53 SSS FUL L25 914 SEA FILE=REGISTRY ABB=ON PLU=ON (L72 OR L73 OR L74 OR L75 L77 OR

QAZI 09/535387

Page 5

L78

G5 Hy CH2G2 O Cy=+G3 G5 Hy CH2G2 O Cy G3 CH N OH 46 45 6 7 8 9 10 @11 12 13

L76)

STR

Ak @28

CH = N - OH

25 26 ОН О CH2-CH-C---O---G4 @19 20 21 22 27

CH2-NH-OH

042 43 44

23 24 ОН О CH2-N-C-NH2 014 15 16 17

33 34 0 Χ CH2-CH-C=---O== G4 @29 30 31 32 35

REP G2 = (0-7) CH2 VAR G3=CHO/NO2/NH2/11/14/19/29/42 VAR G4=H/28 VAR G5=O/S NODE ATTRIBUTES: CONNECT IS E1 RC AT 28 DEFAULT MLEVEL IS ATOM GGCAT IS HIQ AT 45 DEFAULT ECLEVEL IS LIMITED ECOUNT IS M2 N AT 45

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 34

STEREO ATTRIBUTES: NONE

135 SEA FILE=REGISTRY SUB=L77 SSS FUL L78

=> d bib abs hitstr 16-40

ANSWER 16 OF 40 CAPLUS COPYRIGHT 2000 ACS 1993:649760 CAPLUS ΑN

DN 119:249760

Porphyrins coupled with nucleoside bases. Synthesis and characterization ΤI of ether-linked adenine-thymine and guanine-cytosine derivatives

Hisatome, Masao; Ikeda, Koichi; Kishibata, Shusuke; Yamakawa, Koji ΑU

Fac. Pharm. Sci., Sci. Univ. Tokyo, Tokyo, 162, Japan CS

Chem. Lett. (1993), (8), 1357-60 SO CODEN: CMLTAG; ISSN: 0366-7022

DT Journal

LA English

GΙ

Porphyrins I (B = adenine, guanine, thymine, cytosine, R = H; B =AΒ adenine,

R = thyminylbutoxy; B = guanine, R = cytosinylbutoxy) have beensynthesized. Spectroscopic study has revealed that in I [R = O(CH2)4B1] the two nucleic acid bases form inter- and intramol. base pairs in the anti and syn atropisomers, resp., and that the guanine-cytosine pair is closer to the porphyrin ring than the adenine-thymine pair.

Ι

151056-15-4P 151056-16-5P 151056-18-7P IT

RL: SPN (Synthetic preparation); PREP (Preparation)

(intermediate in prepn. of nucleic acid base-contg. porphyrins)

RN 151056-15-4 CAPLUS

CN Benzaldehyde, 2-[4-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)pyrimidinyl)butoxy]- (9CI) (CA INDEX NAME)

RN 151056-16-5 CAPLUS

Benzaldehyde, 2-[4-(4-amino-2-oxo-1(2H)-pyrimidinyl)butoxy]- (9CI) (CA CN INDEX NAME)

$$H_2N$$
 O OHC N (CH_2) $_4$ O

RN 151056-18-7 CAPLUS

Benzaldehyde, 2-[4-(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)butoxy]-CN (9CI)

(CA INDEX NAME)

ANSWER 17 OF 40 CAPLUS COPYRIGHT 2000 ACS L81

ΑN 1993:560277 CAPLUS

DN 119:160277

Preparation of imidazolidinetrione derivatives as intermediates for ulcer TIinhibitors

Matsukubo, Hiroshi; Myashita, Mitsutomo; Koike, Tomozo; Harano, Naoki; IN Maeda, Toshio

PΑ Kyorin Seiyaku Kk, Japan

Jpn. Kokai Tokkyo Koho, 5 pp. SO

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	AP:	PLICATION NO.	DATE
•	JP 05086036 CASREACT 119:160		19930406 ARPAT 119:16027	JP 7	1991-273246	19910925

OS GΙ

ΡI

$$X - A - N$$
 $N - R1$
 OHC
 $O-A-N$
 $N-R1$
 OHC
 OHC

The title compds. [I; R1 = alkyl; A = CH2CH2, propylene, butylene, ΑВ butenylene; X = halo, m-formylphenoxy], intermediates for the antiulcer Searched by John Dantzma 703-308-4488

drug II, are prepd. via, e.g., reaction of urea derivs. X-A-NH-CO-NH-R1 with (COC1)2. E.g., (COC1)2 was added dropwise to C1(CH2)3-NH-CO-NH-Et

CH2Cl2 at .ltoreq.10.degree. and the resulting mixt. was stirred at room temp. for 21 h to give the title compd. 1-(3-chloropropyl)-3-ethylimidazolidinetrione. This when reacted with 3-hydroxybenzaldehyde

in DMF contg. KHCO3 gave antiulcer II.

IT 149911-68-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for ulcer inhibitor)

RN 149911-68-2 CAPLUS

CN Benzaldehyde, 3-[3-(3-ethyl-2,4,5-trioxo-1-imidazolidinyl)propoxy]- (9CI) (CA INDEX NAME)

L81 ANSWER 18 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1990:98478 CAPLUS

DN 112:98478

TI Sodium 2-mercaptoethanesulfonate in reversible adduct formation and water solubilization

AU Rise, Frode; Undheim, Kjell

CS Inst. Chem., Univ. Uppsala, Uppsala, S-751 21, Swed.

SO Acta Chem. Scand. (1989), 43(5), 489-92

CODEN: ACHSE7

DT Journal

LA English

GΙ

Searched by John Dantzma

703-308-4488

AB Sodium 2-mercaptoethanesulfonate (I, coenzyme M) forms 1:1 covalent adducts with high .pi.-electron deficient heterocycles. The addn. is at the thiol function, and the adducts become water sol. as sulfonates. 1H NMR spectroscopy was used to obtain information about electronic and steric effects on the equil. between 2-pyrimidinones and their 1:1

with I. The adducts, e.g., II and III, are potential prodrugs for biol. interesting 2-pyrimidinones.

IT 100944-95-4

RL: RCT (Reactant)
 (addn. reaction of, with sodium mercaptoethanesulfonate, reversibility
and regiochem. of)

- RN 100944-95-4 CAPLUS
- CN Benzaldehyde, 4-[(5-chloro-2-oxo-1(2H)-pyrimidinyl)methoxy]- (9CI) (CA INDEX NAME)

IT 125256-32-8P 125256-42-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and NMR of)

- RN 125256-32-8 CAPLUS
- CN Ethanesulfonic acid, 2-[[5-chloro-1-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-4-pyrimidinyl]thio]-, monosodium salt (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HO}_3\text{S} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{S} & \overset{\text{H}}{\text{N}} & \text{O} \\ & & \text{CH}_2\text{-}\text{O} \end{array}$$

- Na
- RN 125256-42-0 CAPLUS
- CN Ethanesulfonic acid, 2-[[5-chloro-3-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-4-pyrimidinyl]thio]-, monosodium salt (9CI) (CA INDEX NAME)

Na

L81 ANSWER 19 OF 40 CAPLUS COPYRIGHT 2000 ACS

1990:77145 CAPLUS

DN 112:77145

A cage compound derived from cyclotriveratrylene and diphenylglycoluril TΙ subunits

Smeets, J. W. H.; Coolen, H. K. A. C.; Zwikker, J. W.; Nolte, R. J. M. ΑU

CS Dep. Org. Chem., Univ. Utrecht, Utrecht, 3584 CH, Neth.

Recl. Trav. Chim. Pays-Bas (1989), 108(6), 215-18 SO CODEN: RTCPA3; ISSN: 0165-0513

DT Journal

LA English

OS CASREACT 112:77145

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- Title compd. I was prepd. as a mixt. of stereoisomers in 4 steps from vanillin. Monoetherification of vanillin with Br(CH2)6Br and exhaustive alkylation of diphenylglycoluril with the adduct thus prepd. gave diphenyltetrakis[(aryloxy)hexyl]glycoluril II. NaBH4 redn. of II, followed by high-diln. cyclotrimerization of the reduced product in HCO2H contg. Me2NCHO gave 31% I. I has a well defined cavity and a free functionalized arm.
- ΙT 125232-26-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and redn. of, with sodium borohydride)

125232-26-0 CAPLUS RN

CNBenzaldehyde,

4,4',4'',4'''-[(dihydro-2,5-dioxo-3a,6a-diphenylimidazo[4,5-

d]imidazole-1,3,4,6(2H,5H)-tetrayl)tetrakis(6,1-hexanediyloxy)]tetrakis[3methoxy- (9CI) (CA INDEX NAME)

L81 ANSWER 20 OF 40 CAPLUS COPYRIGHT 2000 ACS

ΑN 1989:189240 CAPLUS

110:189240 DN

Synthesis and antibacterial activity of some new 2-aryloxymethyl-3-TIsubstituted-quinazolin-4(3H)-ones

ΑU Khan, A.; Saksena, R. K.

CS D. A. V. Coll., Kanpur Univ., Kanpur, India

SO Pharmazie (1988), 43(12), 864-5 CODEN: PHARAT; ISSN: 0031-7144

DT Journal

LAEnglish

Halogenated quinazolinones were synthesized, and 2-aryloxymethyl-3-AB arylquinazolin-4(3H)-ones and 2-aryloxymethyl-3-(2-substituted ethyl)quinazolin-4(3H)-ones were screened for antibacterial activity. Most compds. in each group showed some activity.

ΙT 120244-20-4P 120244-25-9P 120244-29-3P 120244-30-6P 120268-13-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and antibacterial activity of)

RN 120244-20-4 CAPLUS

CN 4(3H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]-3-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 120244-25-9 CAPLUS

4(3H)-Quinazolinone, 3-(4-methylphenyl)-2-[(4-nitrophenoxy)methyl]- (9CI) CN (CA INDEX NAME)

RN 120244-29-3 CAPLUS

CN 4(3H)-Quinazolinone, 3-(2-chloroethyl)-2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

RN 120244-30-6 CAPLUS

CN 4(3H)-Quinazolinone, 3-(2-fluoroethyl)-2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

RN 120268-13-5 CAPLUS

CN 4(3H)-Quinazolinone, 3-(2-hydroxyethyl)-2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

IT 120244-31-7

RL: RCT (Reactant)

(reaction of, with aminoethanol)

RN 120244-31-7 CAPLUS

CN 4(1H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

$$\bigcap_{N}^{H} \bigcap_{N \to \infty} CH_2 - O - \bigcap_{N \to \infty} O$$

L81 ANSWER 21 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1988:437790 CAPLUS

DN 109:37790

TI Sulfonic and phosphonic acids formed by bisulfite and phosphite adduct formation with pyrimidinones

AU Benneche, Tore; Strande, Per; Undheim, Kjell CS Dep. Chem., Univ. Oslo, Oslo, N-0315, Newson

CS Dep. Chem., Univ. Oslo, Oslo, N-0315, Norway SO Acta Chem. Scand., Ser. B (1987), B41(6), 448-54

CODEN: ACBOCV; ISSN: 0302-4369

DT Journal LA English

OS CASREACT 109:37790

GΙ

Alkylation of pyrimidinone I (R = H) with ClCHR1R2 [R1 = H, Me, Ph; R2 = OPh, substituted PhO, N(CO2Et)CH2Ph, SC6H4Cl-4, SCH2Ph, 2-naphthyloxy] gave N- and O-alkylated products I (R = CHR1R2) and II. Sulfurization of I (R = CHR1R2) gave pyrimidines III (R3 = SO3Na) as well as 3,6-bisulfites. Phosphorylation of I (R = CH2Ph, CH2OCH2C6H4Cl-4) gave regiospecifically III (R1 = H; R2 = Ph, OCH2C6H4Cl-4; R3 = PO3H2) via hydrolysis.

IT 100944-58-9P 100944-59-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and desulfurization of)

RN 100944-58-9 CAPLUS

CN 4-Pyrimidinesulfonic acid, 5-chloro-1-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Searched by John Dantzma 703-308-4488

QAZI 09/535387

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(9CI) (CA INDEX NAME)

=> d bib abs hitstr 15

L81 ANSWER 15 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1994:106638 CAPLUS

DN 120:106638

TI The synthesis of a potential anti-cancer agent containing the caffeine and

1,2,3-benzotriazine moieties

AU Parrick, John; Mehta, Lina K.; Hodgkiss, Richard J.

CS Dep. Chem., Brunel Univ., Uxbridge/Middlesex, UB8 3PH, UK

SO J. Heterocycl. Chem. (1993), 30(2), 323-7

CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 120:106638

GΙ

AB The potential anti-cancer agent I has been synthesized from 4-(4-chlorobutoxy)-2-nitroaniline via benzotriazine N-oxide II. Theophylline has been reacted with II to give the N-oxide, which was oxidized to I. I has been found to be ineffective as a radiosensitizer. IT 152538-23-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and oxidn. of)

RN 152538-23-3 CAPLUS

CN 1H-Purine-2,6-dione, 7-[4-[(3-amino-4-oxido-1,2,4-benzotriazin-7-yl)oxy]butyl]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

ΙT 152538-24-4P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as anticancer agent)

RN 152538-24-4 CAPLUS

1H-Purine-2,6-dione, 7-[4-[(3-amino-1,4-dioxido-1,2,4-benzotriazin-7-CN yl)oxy]butyl]-3,7-dihydro-1,3-dimethyl- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

• Na

RN 100944-59-0 CAPLUS

CN 4-Pyrimidinesulfonic acid, 5-chloro-3-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)

● Na

IT 100944-95-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and sulfurization of, with bisulfites)

RN 100944-95-4 CAPLUS

CN Benzaldehyde, 4-[(5-chloro-2-oxo-1(2H)-pyrimidinyl)methoxy]- (9CI) (CA INDEX NAME)

L81 ANSWER 22 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1988:123961 CAPLUS

DN 108:123961

- TI DNA-nitrosourea interactions. High-performance liquid chromatography of cross-linked dinucleosides and substituted deoxynucleosides
- AU Maggio, A. F.; Pompon, A.; Lucas, M.; Barascut, J. L.; Imbach, J. L.
- CS Lab. Chim. Bio-Organ., Univ. Sci. Tech., Montpellier, 34060, Fr.

SO J. Chromatogr. (1988), 436(1), 23-30 CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

A reconstituted mixt. of 5 cross-linked dinucleosides possibly involved AΒ

in

DNA-nitrosourea interactions, and of their degrdn. products (nucleobases, deoxynucleosides and mono- or disubstituted deoxynucleosides), was analyzed by reversed-phase HPLC using C18 columns and a diode-array detector. The chromatog. conditions for sepg. the 21 investigated compds.

were optimized, and the compds. were identified by both their retention times and their UV spectra. A structure-retention time relationship was obsd. under suitable conditions and is discussed. Its validity was confirmed by the prediction of the retention time of a cross-linked dinucleoside synthesized for this purpose.

111447-28-0 111447-29-1 ΤТ

RL: ANT (Analyte); ANST (Analytical study) (detn. of, by HPLC, in reconstructed mixt. of cross-linked dinucleosides and their degrdn. products)

RN 111447-28-0 CAPLUS

Guanosine, 2'-deoxy-6-0-[2-[3-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-CN 3,6-dihydro-2,6-dioxo-1(2H)-pyrimidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111447-29-1 CAPLUS

Guanosine, 2'-deoxy-6-0-[2-[3-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-CN 3,6-dihydro-6-imino-2-oxo-1(2H)-pyrimidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L81 ANSWER 23 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1987:637188 CAPLUS

DN 107:237188

TI Regioselective synthesis of linked dinucleosides: reaction mechanism of nitrosoureas

AU Maggio, A. F.; Lucas, M.; Barascut, J. L.; Pompon, A.; Imbach, J. L.

CS Lab. Chim. Bio-Org., Univ. Sci. Tech. Languedoc, Montpellier, 34060, Fr.

SO Nouv. J. Chim. (1986), 10(11), 643-50 CODEN: NJCHD4; ISSN: 0398-9836

DT Journal

LA French

OS CASREACT 107:237188

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Linked dinucleosides were regioselectively prepn. by linking deoxyguanosine (I), deoxycytidine, (II), and deoxyuridine synthons. E.q.,

the condensation of synthon III of I with synthon IV of II and deprotection gave the guanosylcytidylethane V.

IT 111447-28-0P 111447-29-1P

RN 111447-28-0 CAPLUS

CN Guanosine, 2'-deoxy-6-Q-[2-[3-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-3,6-dihydro-2,6-dioxo-1(2H)-pyrimidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111447-29-1 CAPLUS

CN Guanosine, 2'-deoxy-6-O-[2-[3-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-3,6-dihydro-6-imino-2-oxo-1(2H)-pyrimidinyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L81 ANSWER 24 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1986:129922 CAPLUS

DN 104:129922

TI Pyrimidinone derivatives

IN Undheim, Kjell; Benneche, Tore

PA Nyegaard og Co. A/S, Norway

SO Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

Searched by John Dantzma

703-308-4488

DT Patent LA English FAN.CNT 1

FAN.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 160573 EP 160573	АЗ	19851106 19861120	EP 1985-303102	19850501
PRAI GI	R: AT, BE, NO 8501714 DK 8501970 JP 61010562 GB 1984-11291	A A	19851104 19851103 19860118	LI, LU, NL, SE NO 1985-1714 DK 1985-1970 JP 1985-93948	19850430 19850502 19850502

R1 C1 NCHR2X(CR4R5)
$$_{n}$$
R3 NaO3S NCH2O CHO

I SO3Na NCH2O CHO

NCH2O CHO

III

Bisulfite addn. products of pyrimidinones I [R1 = CF3, halo; R2 = H, alkyl, alkanoyl, Ph; R3 = (un)substituted arom., heteroarom.; R4, R5 = H, alkyl; X = O, S, R6N; R6 = CHO, alkanoyl, alkoxycarbonyl; n = 0, 1], useful as neoplasm inhibitors (no data), were prepd. Thus, 4-HOC6H4CHO was alkylated with MeSCH2Cl to give 4-MeSCH2OC6H4CHO which was treated with SO2Cl2 to give 4-ClCH2OC6H4CHO. The latter was treated with 5-chloro-2(1H)-pyrimidinone-HCl to give I (R1 = Cl, R2 = H, R3 = 4-OCHC6H4, X = O, n = 0) which was stirred at room temp. in aq. NaHSO3 to give isomeric bisulfite addn. products II and III.

100944-94-3P 100944-95-4P 100945-07-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and addn. reaction of, with sodium bisulfite)
RN 100944-94-3 CAPLUS

CN 2(1H)-Pyrimidinone, 5-chloro-1-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

RN 100944-95-4 CAPLUS

CN Benzaldehyde, 4-[(5-chloro-2-oxo-1(2H)-pyrimidinyl)methoxy]- (9CI) (CA INDEX NAME)

RN 100945-07-1 CAPLUS

CN Benzaldehyde, 4-[[2-oxo-5-(trifluoromethyl)-1(2H)-pyrimidinyl]methoxy]-(9CI) (CA INDEX NAME)

IT 100944-58-9P 100944-59-0P 100944-64-7P 100944-65-8P 100944-67-0P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as neoplasm inhibitor)

RN 100944-58-9 CAPLUS

CN 4-Pyrimidinesulfonic acid, 5-chloro-1-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 100944-59-0 CAPLUS

CN 4-Pyrimidinesulfonic acid, 5-chloro-3-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Na

RN 100944-64-7 CAPLUS
CN 4-Pyrimidinesulfonic acid,
1-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro2-oxo-5-(trifluoromethyl)-, monosodium salt (9CI) (CA INDEX NAME)

• Na

RN 100944-65-8 CAPLUS
CN 4-Pyrimidinesulfonic acid,
3-[(4-formylphenoxy)methyl]-1,2,3,4-tetrahydro2-oxo-5-(trifluoromethyl)-, monosodium salt (9CI) (CA INDEX NAME)

● Na

RN 100944-67-0 CAPLUS
CN 4-Pyrimidinesulfonic acid, 5-chloro-1,2,3,4-tetrahydro-1-[(4-nitrophenoxy)methyl]-2-oxo-, monosodium salt (9CI) (CA INDEX NAME)

Na

L81 ANSWER 25 OF 40 CAPLUS COPYRIGHT 2000 ACS

ΑN 1983:179330 CAPLUS

DN 98:179330

Reaction of quinoxaline derivatives with nucleophilic reagents TI

Badr, Mahmoud Zarif Amin; El-Naggar, Galal Mohamed; El-Sherief, Hassan Ahmad Hassan; Abdel-Rahman, Abdou El-Sayed; Aly, Moustafa Fouzy

CS Fac. Sci., Assiut Univ., Assiut, Egypt

SO Bull. Chem. Soc. Jpn. (1983), 56(1), 326-30

CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Treatment of 2-chloro-3-methylquinoxaline with arom. amines in basic AΒ medium gave aminoquinoxalines \bar{I} (R = H, Me, Cl) and with HSCH2CO2H gave thioether II. Condensation of 3-methyl-2(1H)-quinoxalinone with arom. aldehydes gave styrylquinoxalines III (R1 = H, Me, Me2N, C1, HO, NO2) which added Br2 in HOAc to give dibromo derivs. which reacted with morpholine, NaOMe, and piperidine to give phenethylquinoxalines IV (R1 =4-MeO, R2 = morpholino; R1 = 4-No2, R2 = MeO) and V. 3-(Bromomethyl)-2(1H)-quinoxalinone underwent nucleophilic substitution with arom. amines,

Na saccharine, and K phthalimide, and 3-methyl-2(1H)-quinoxalinethione underwent S-alkylation, by Me2SO4 and ClCH2CO2H and BrCH2CH2CO2H.

IT85516-32-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

85516-32-1 CAPLUS RN

2(1H)-Quinoxalinone, 3-[(4-nitrophenoxy)methyl]- (9CI) (CA INDEX NAME)

ANSWER 26 OF 40 CAPLUS COPYRIGHT 2000 ACS

ΑN 1983:72028 CAPLUS

DN 98:72028

Some new 2-aryloxymethyl-3-.alpha.-substituted carboxymethyl-6,8-TIsubstituted 4-quinazolones as possible anticonvulsants

Husain, M. I.; Singh, Eira ΑU

Chem. Dep., Lucknow Univ., Lucknow, India CS

Pharmazie (1982), 37(6), 408-10 SO CODEN: PHARAT; ISSN: 0031-7144

DTJournal LA English

GΙ

$$R^2$$
 R^3
 CH_2O
 R^1
 I

The title compds. I (R = 3,4-Me2, p-O2N, H, p-Me, o-Cl; R2 = H, Br; R3 = HAΒ Η,

Br, iodo, R4 = H, PhCH2, Me, imidazolylmethyl Me2CH, H2CC(:NH)NH(CH2)3, MeCEt, Me2CHCH2, H2NCOCH2CH2) were prepd. by treating the anthranils II with H2NCHR4CO2H. Most I gave 20-60% anticonvulsant protection against pentylenetetrazole induced seizures. The monoamine oxidase activity of I was also reported.

ΙT 83793-67-3P 83793-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 83793-67-3 CAPLUS

3(4H)-Quinazolineacetic acid, 8-iodo-2-[(4-nitrophenoxy)methyl]-4-oxo-CN (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} I & & \\ N & CH_2-O \\ N & CH_2-CO_2H & NO_2 \end{array}$$

RN 83793-68-4 CAPLUS

CN 3(4H)-Quinazolineacetic acid, .alpha.-(1-methylethyl)-2-[(4-nitrophenoxy)methyl]-4-oxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 83793-69-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., anticonvulsant, and monoamine oxidase activity of)

RN 83793-69-5 CAPLUS

CN 3(4H)-Quinazolineacetic acid, .alpha.-(1H-imidazol-1-ylmethyl)-2-[(4-nitrophenoxy)methyl]-4-oxo-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L81 ANSWER 27 OF 40 CAPLUS COPYRIGHT 2000 ACS

AN 1980:620689 CAPLUS

DN 93:220689

TI Synthesis of 2-phenoxymethyl-3-(2'-pyridyl/thiazolyl)-4-quinazolones as possible antifertility drugs

AU Shukla, J. S.; Ahmad, I.

CS Dep. Chem., Univ. Lucknow, Lucknow, India

SO Indian J. Chem., Sect. B (1979), 17B(6), 651-2

CODEN: IJSBDB; ISSN: 0376-4699

DT Journal LA English

GΙ

$$R^{1}$$
 N^{1}
 R^{2}
 R^{2}
 R^{2}
 R^{1}
 R^{2}

2-Phenoxymethyl-3-(2-pyridyl/thiazolyl)-4-quinazolones I (R = H, Me, NO2, AВ OMe; R1 = H, Br, iodo; R2 = H, Br; R3 = 2-pyridyl, 2-thiazolyl) were prepd. by cyclization of the substituted anthranilic acids with phenoxyacetyl chlorides followed by condensation with R3NH2.

ΙT 73342-54-8P 73342-55-9P 75543-04-3P 75543-05-4P 75543-06-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

73342-54-8 CAPLUS RN

4(3H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]-3-(2-pyridinyl)- (9CI) CN (CA INDEX NAME)

$$N$$
 CH_2-O
 N
 N
 R
 NO_2

RN 73342-55-9 CAPLUS

4(3H)-Quinazolinone, 2-[(4-nitrophenoxy)methyl]-3-(2-thiazolyl)- (9CI) CN (CA INDEX NAME)

RN 75543-04-3 CAPLUS

CN 4(3H)-Quinazolinone, 6-bromo-2-[(4-nitrophenoxy)methyl]-3-(2-thiazolyl)-(9CI) (CA INDEX NAME)

RN 75543-05-4 CAPLUS

CN 4(3H)-Quinazolinone, 6,8-dibromo-2-[(4-nitrophenoxy)methyl]-3-(2-thiazolyl)- (9CI) (CA INDEX NAME)

RN 75543-06-5 CAPLUS

CN 4(3H)-Quinazolinone, 6,8-dibromo-2-[(4-nitrophenoxy)methyl]-3-(2-pyridinyl)- (9CI) (CA INDEX NAME)